Atomic and Molecular Data Activities at NIFS in 2015 – 2017

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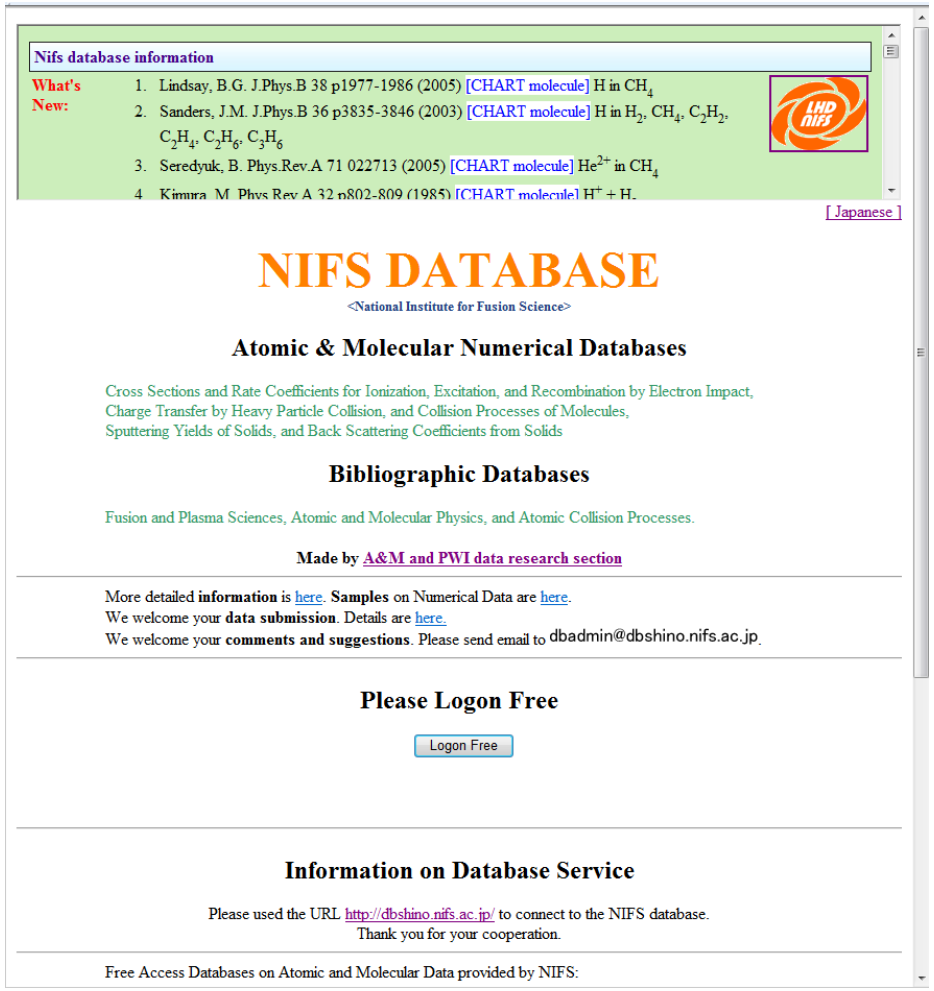
Outline

1. NIFS database
2. Satellite databases
3. Research activities related to AM data
4. Concluding remarks

1. NIFS database

http://dbshino.nifs.ac.jp/



Retrievable numerical database for collision processes

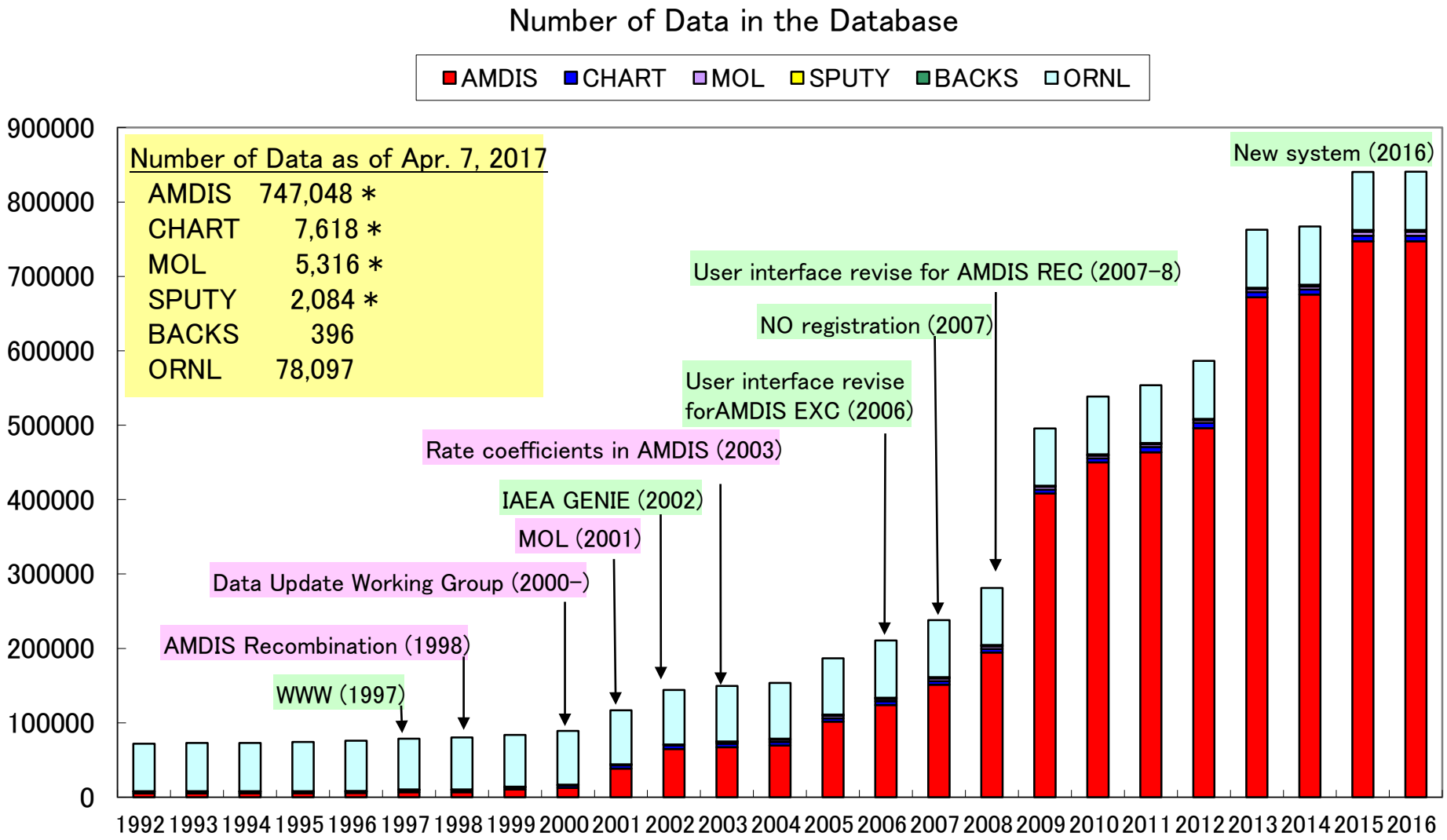
Recent changes

- Database managing system is changed from Oracle to PostgreSQL and the whole system was rebuilt in 2016.
- New functions are added.
- New “simple search” entry pages are available for all sub databases.
- Some bugs in BACKS displaying system are fixed.
- New data added for AMDIS, CHART, AMOL, and CMOL.

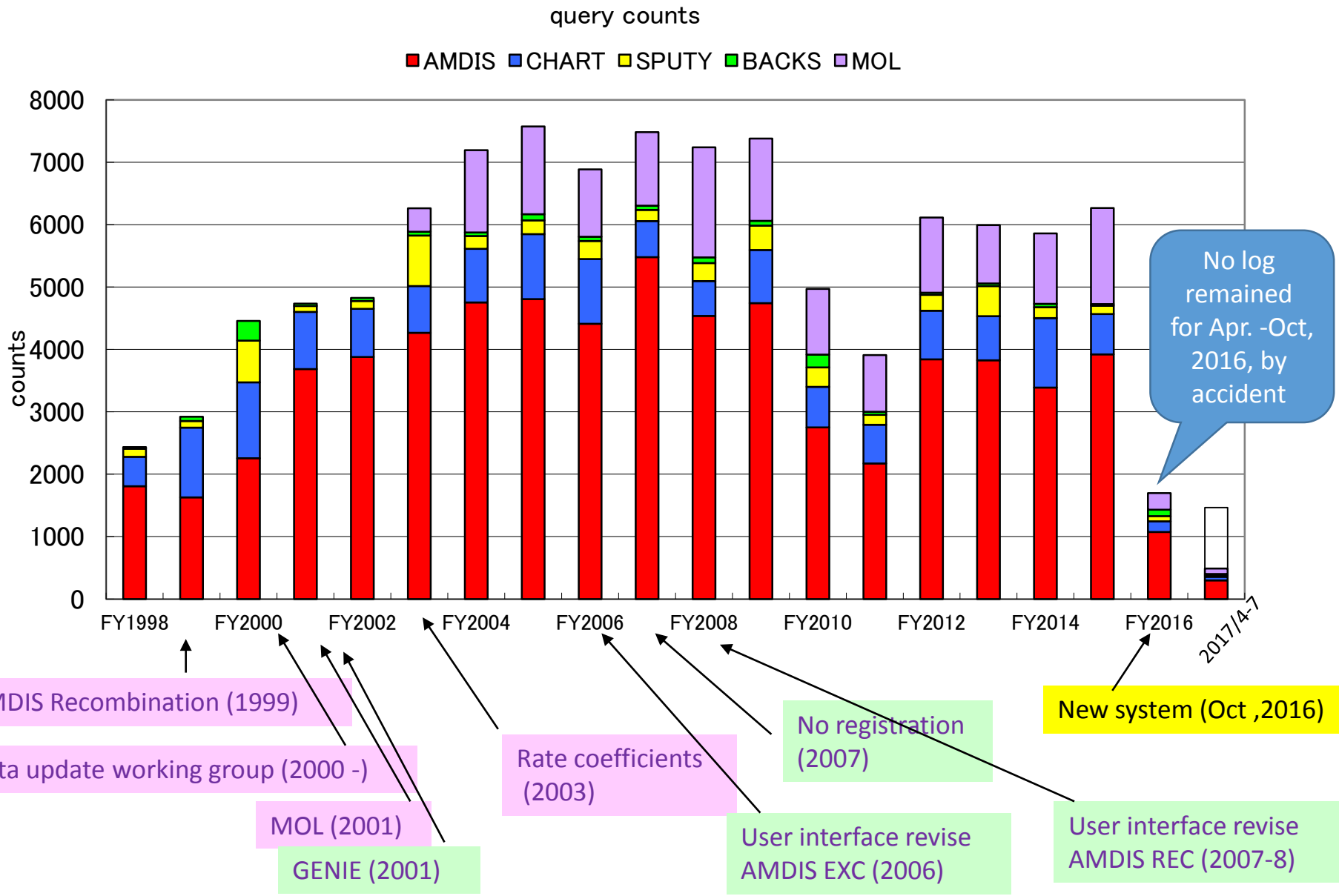
AM and PWI Numerical Database (http://dbshino.nifs.ac.jp)

DB Name		Contents	Period	Records (Aug.3, 2017)
AMDIS	EXC	Electron impact excitation of atoms	1961–2015	**755,321** (747,001; Oct. 2015)
	ION	Electron impact ionization of atoms		
	DIO	Electron impact dissociation of simple molecules		
	REC	Electron recombination of atoms		
CHART		Charge exchange of ion–atom collision	1957–2013	**7,618** (7,616)
AMDIS MOL (AMOL)		Electron collision with molecules	1956–2015	**5,326** (5,295)
CHART MOL (CMOL)		Heavy particle collision with molecules		
SPUTY		Sputtering yield of solid	1931–2007	2,084 (2,084)
BACKS		Reflection coefficient of solid surface	1976–2002	396 (396)
(AM Bibliographic database)				
ORNL		Bibliography on atomic collisions collected at ORNL, USA	1959–2009	78,097

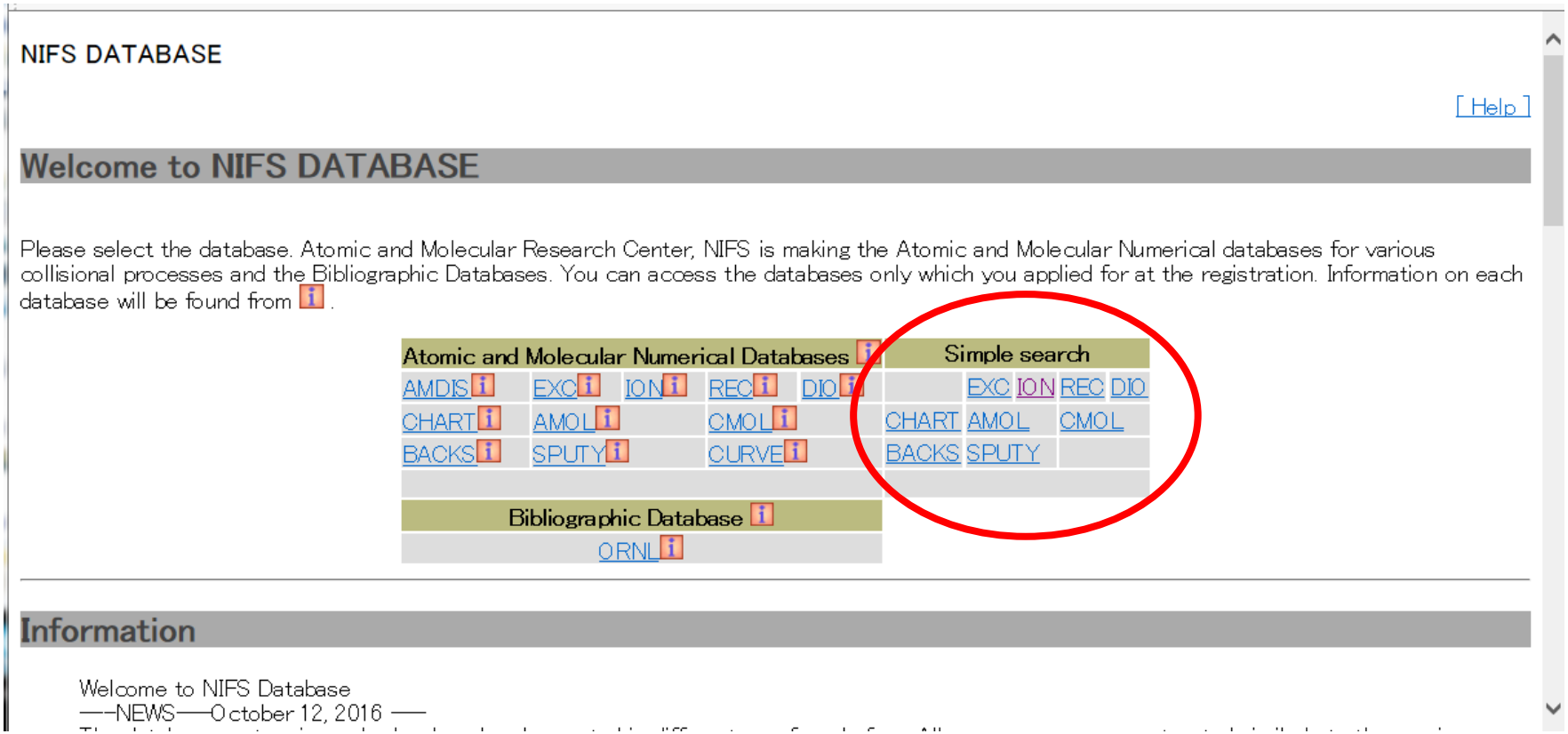
Change of number of data recodes in the database



Access counts to the database (query counts)

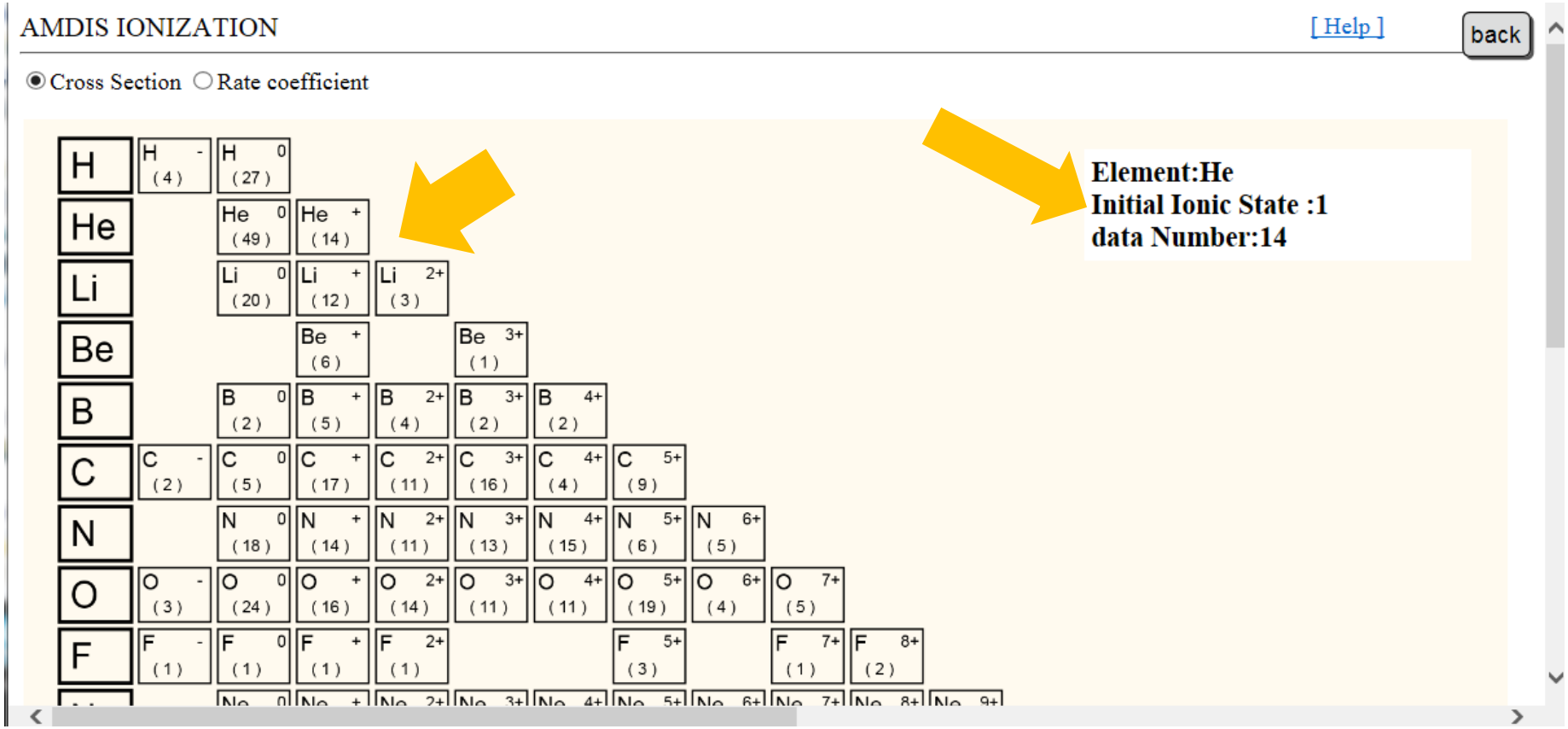


New “simple search” entries for each sub database



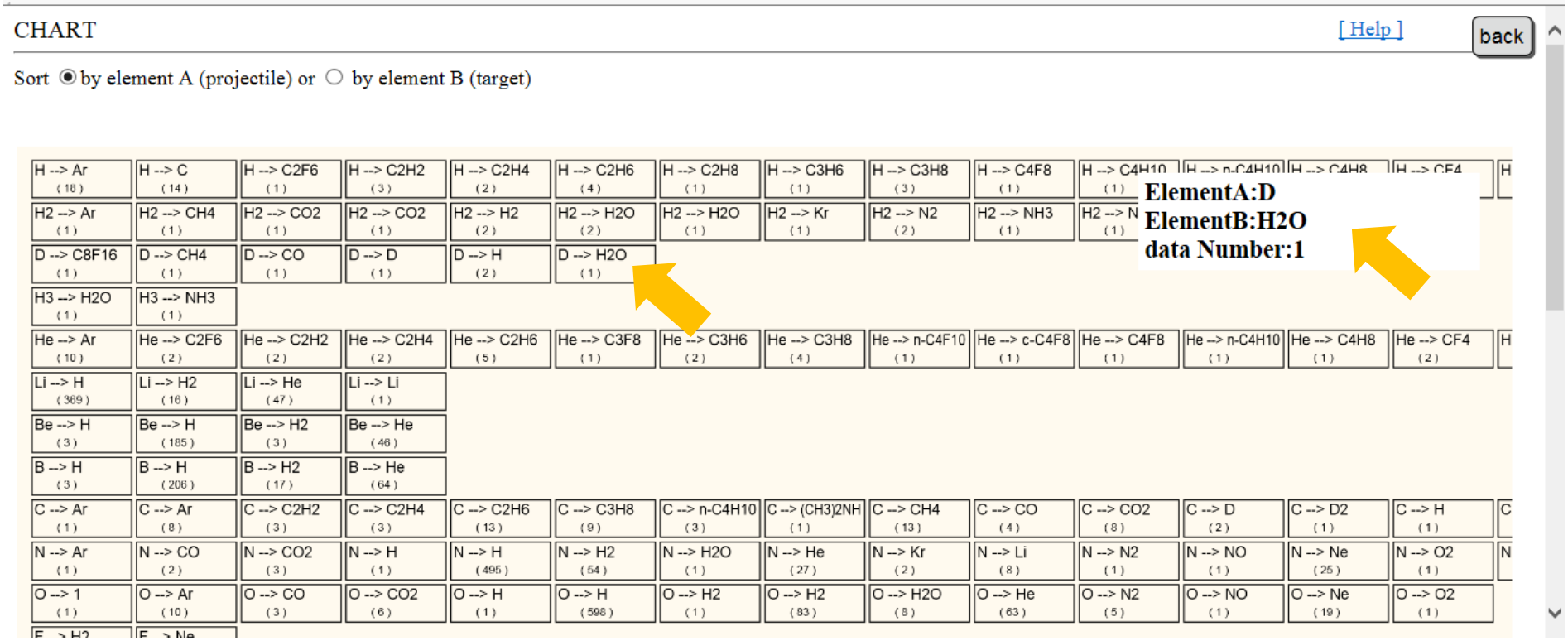
- Easy to select initial ionic state / projectile and target elements.
- Especially, it is easy to find molecules in the databases.
- Total number of data records in the databases are shown.

New “simple search”



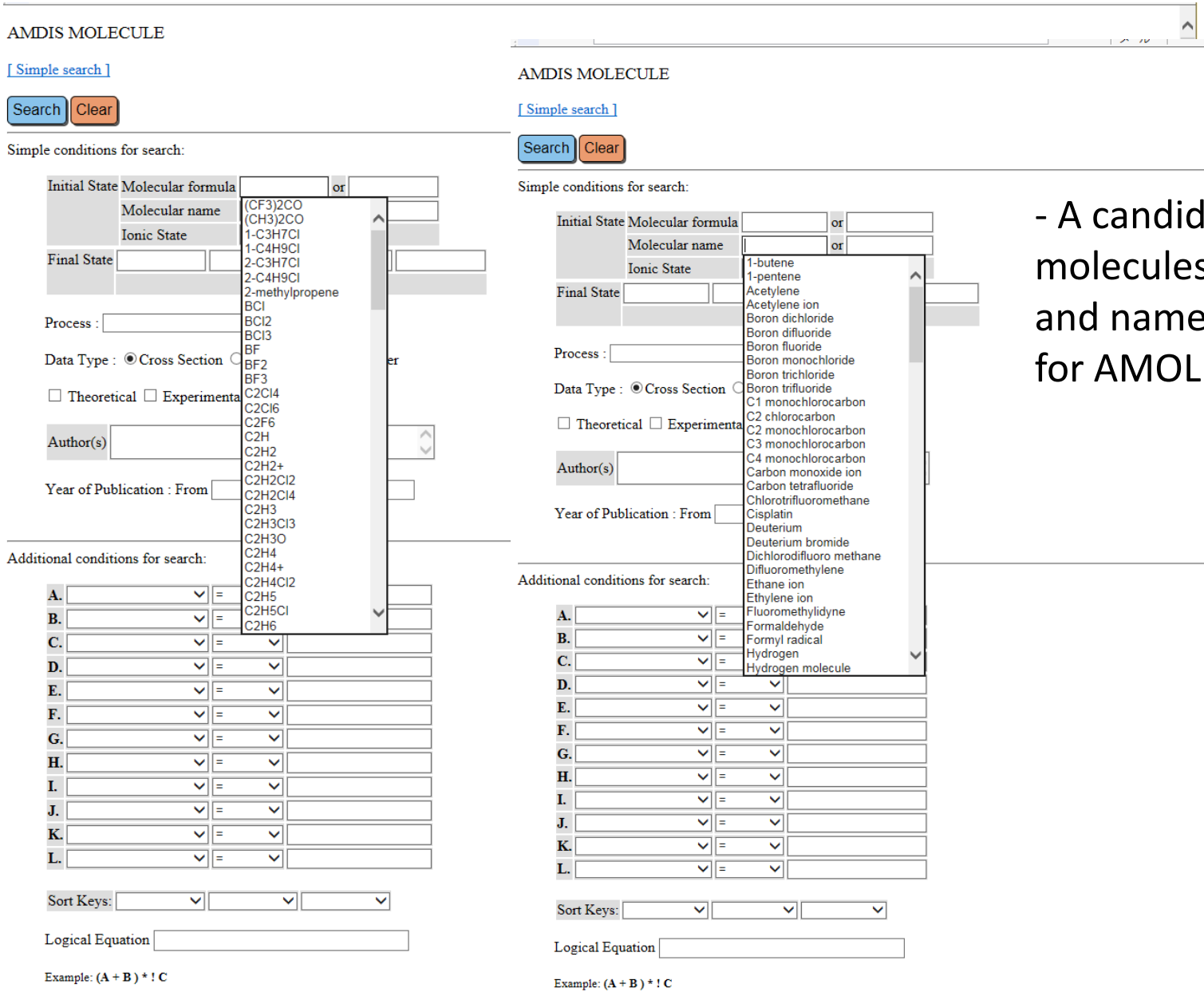
- Users can select an initial ionic state from the table matrices for ION, EXC, REC, and AMOL.
- The table can expand to see well.
- The matrix is built dynamically from the data tables in the database.

New “simple search”



- Initial projectile and target elements are shown as matrix element for selection for CHART, CMOL, SPUTY and BACKS.

New function

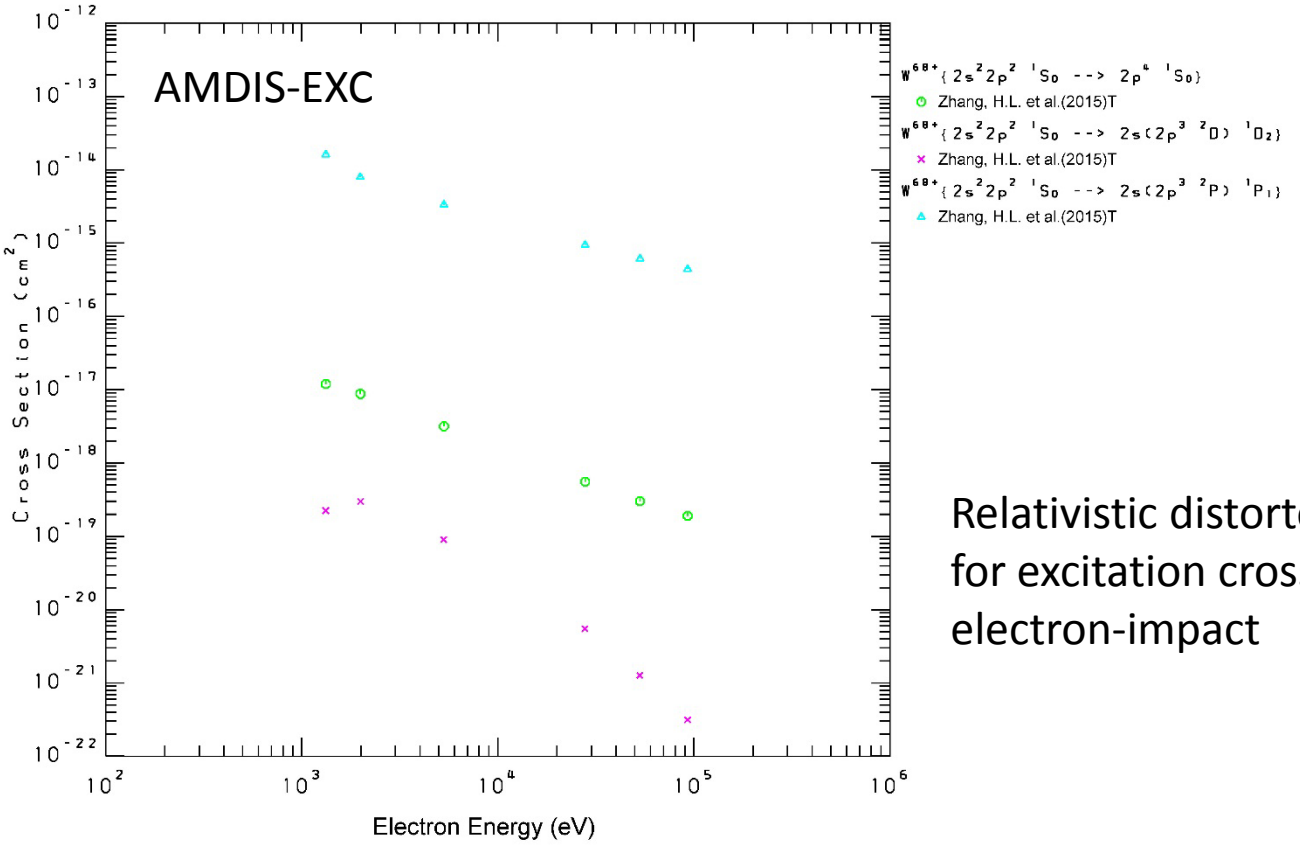


- A candidate list of molecules for formula and name are shown for AMOL and CMOL.

Working group for data update

- Working group has been organized to update data with Japanese atomic and molecular physicists.
- Main targets to search data of last two years tungsten and heavy elements (FY2015 -).
- New data on heavy elements have been searched for update.

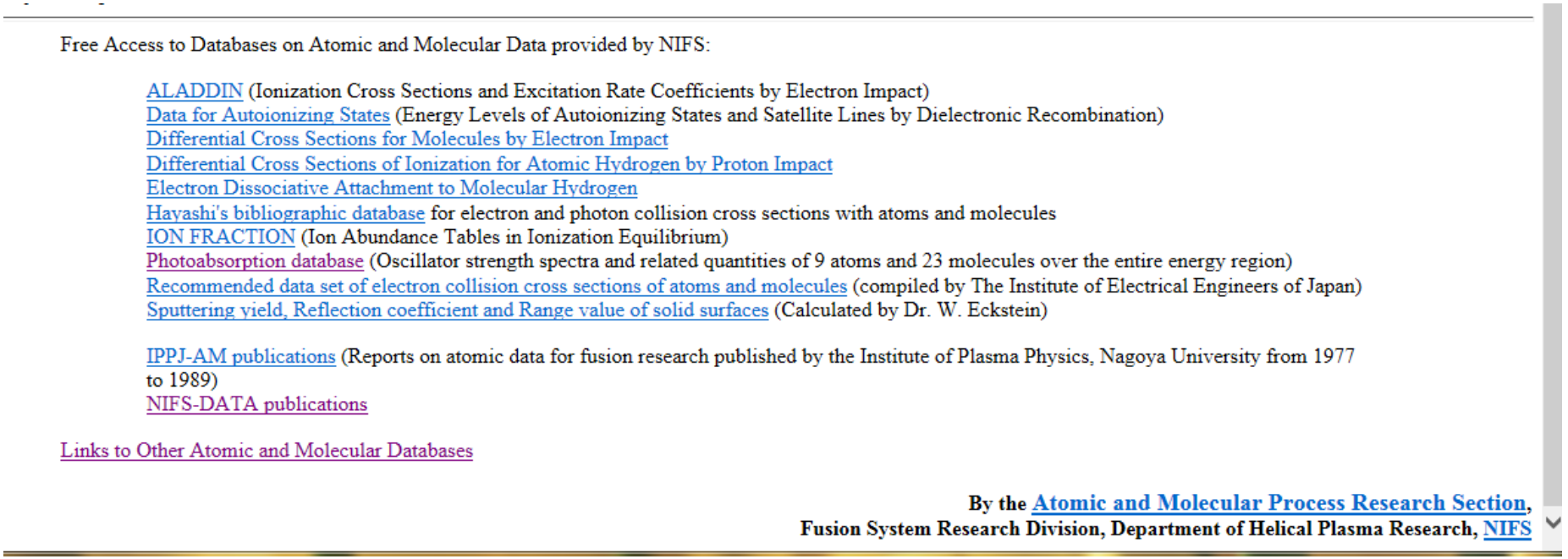
Examples of newly registered data



Relativistic distorted-wave calculations for excitation cross sections by electron-impact

Excitation cross sections for 26 ≦Z≦92 B-like, C-like, N-like, O-like ions
By C. J. Fontes & H. L. Zhang, ADNDT 100 (2014) 802; ADNDT 100 (2014) 1292, ADNDT 101 (2015) 143; H. L .Zhang & C. J. Fontes, ADNDT 101 (2015) 41

2. Satellite databases



Free Access to Databases on Atomic and Molecular Data provided by NIFS:

ALADDIN (Ionization Cross Sections and Excitation Rate Coefficients by Electron Impact)
Data for Autoionizing States (Energy Levels of Autoionizing States and Satellite Lines by Dielectronic Recombination)
Differential Cross Sections for Molecules by Electron Impact
Differential Cross Sections of Ionization for Atomic Hydrogen by Proton Impact
Electron Dissociative Attachment to Molecular Hydrogen
Hayashi's bibliographic database for electron and photon collision cross sections with atoms and molecules
ION FRACTION (Ion Abundance Tables in Ionization Equilibrium)
Photoabsorption database (Oscillator strength spectra and related quantities of 9 atoms and 23 molecules over the entire energy region)
Recommended data set of electron collision cross sections of atoms and molecules (compiled by The Institute of Electrical Engineers of Japan)
Sputtering yield, Reflection coefficient and Range value of solid surfaces (Calculated by Dr. W. Eckstein)

IPPJ-AM publications (Reports on atomic data for fusion research published by the Institute of Plasma Physics, Nagoya University from 1977 to 1989)
NIFS-DATA publications

Links to Other Atomic and Molecular Databases

By the Atomic and Molecular Process Research Section,
Fusion System Research Division, Department of Helical Plasma Research, NIFS

- Various small databases are linked at the database top page, such as rate coefficients of electron dissociative attachment to molecular hydrogen.

- No new entries during last 2 years

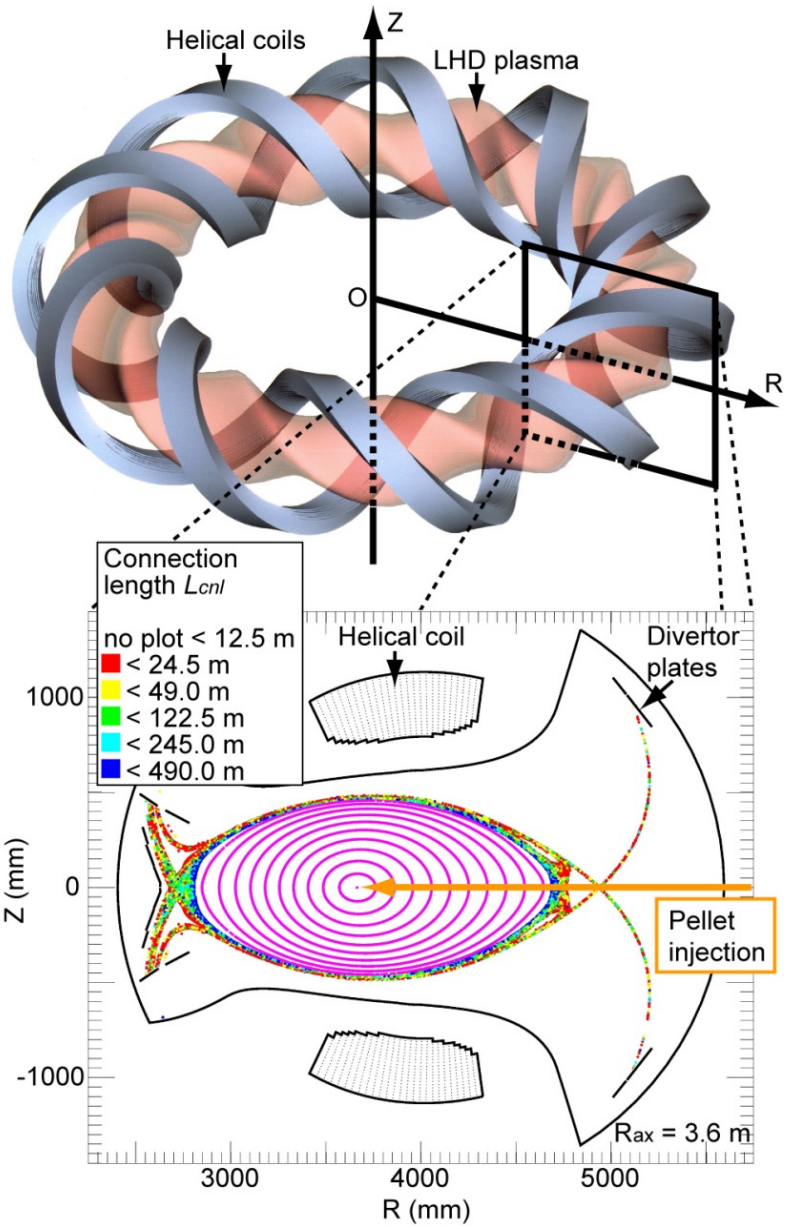
3. Research activities related to AM data under collaboration

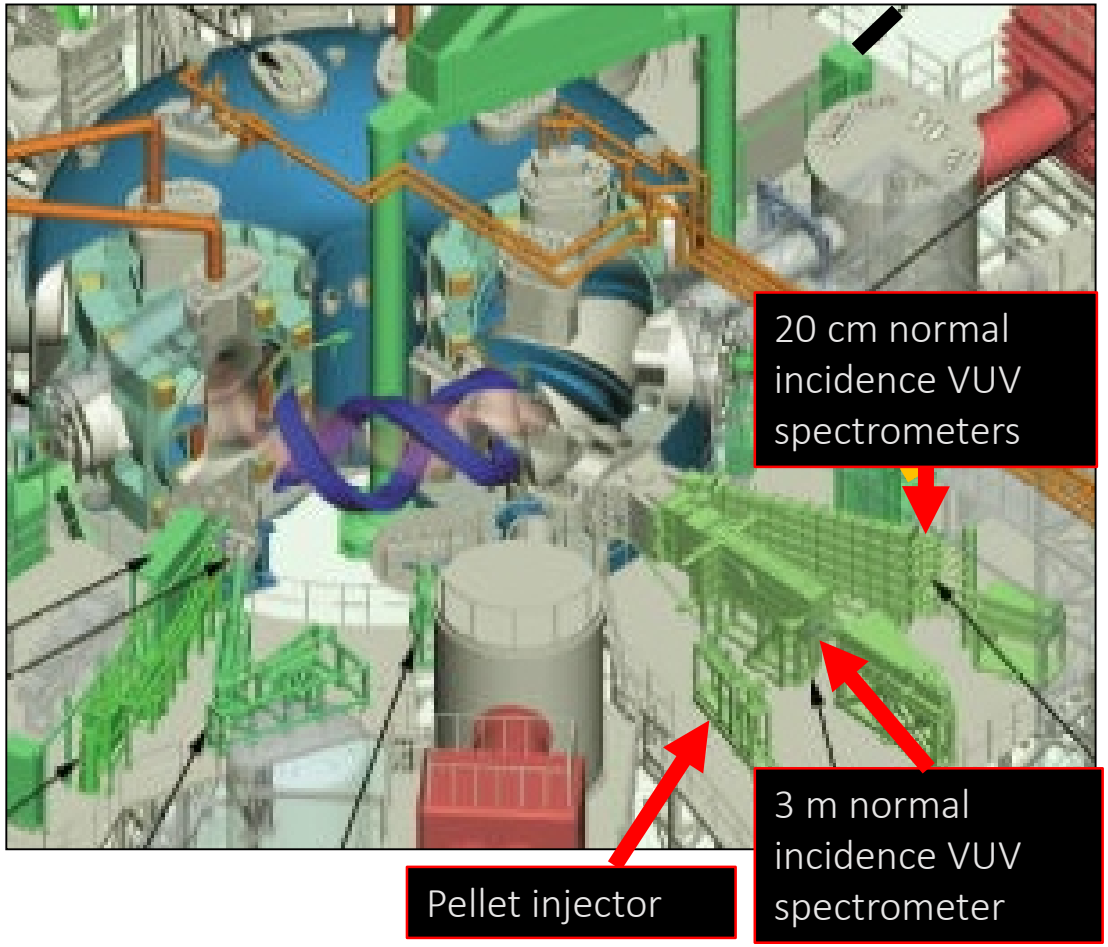
- Experimental and theoretical study on tungsten ions have been carried out continuously.
- EUV and visible spectra of Tungsten ions measured with Tokyo-EBIT, CoBIT, and LHD.
- Atomic data calculations and CR model constructed for Tungsten ions have been conducted to compare with spectra.

- EUV spectra measurements of high Z elements such as lanthanides, tungsten, and bismath with LHD have been done.
- Atomic structure and opacity calculations on low-charged high Z elements are on going for astrophysical purpose.
- Isotope effect in dissociation processes of deuterated molecules from doubly excited states are studied.

Experiments with Large Helical Device

- **Toroidal magnetic field < 3 T**
- **Major radius = 3.6 m**
- **Averaged minor radius = 0.64 m**
- **Toroidal period number = 10**
- **Poloidal mode number = 2**

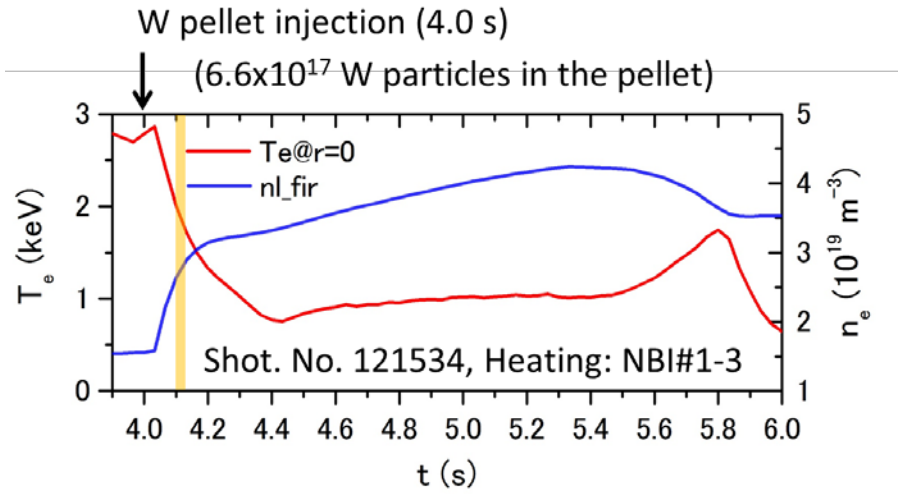




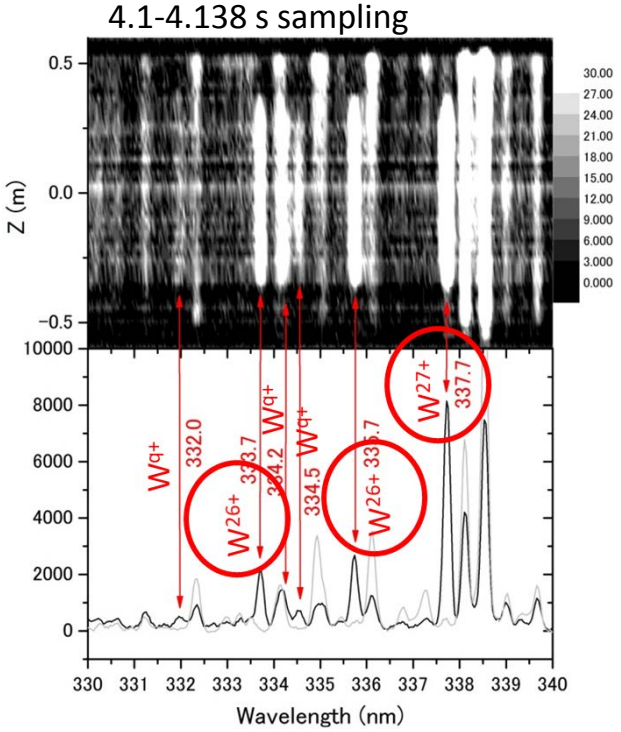
3.1 Observation of ground-state M1 lines of W^{q+} HCI in LHD core plasmas and its application to ion density analysis

D. Kato et al., IAEA FEC2016.

Visible and near-UV emission lines of tungsten ions are useful for analysis of tungsten ion distributions at ITER because the radiation shielding of detectors is not basically necessary by using optical fibers.



11 visible lines of W^{q+} identified in 330 – 390 nm

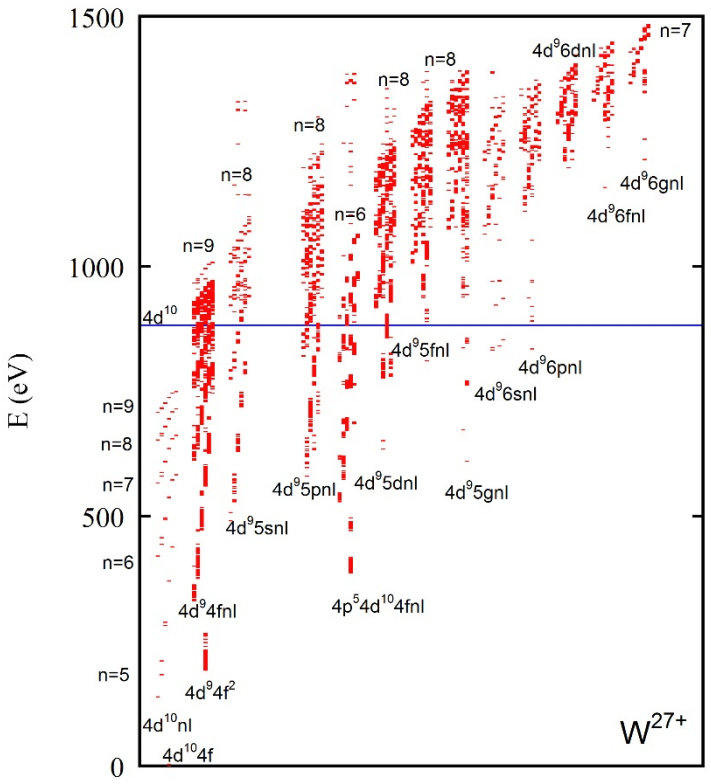


q+	gr	upper	lower	LHD	EBIT	MCDF	RMBPT
27+	4f	$^2F_{7/2}$	$^2F_{5/2}$	337.73(2)	337.743(26)	339.3 338.18	338.4
26+	$4f^2$	$^3F_4$	$^1G_4$	335.73(2)	335.758(11)		
			$^3F_3$	333.70(2)	333.748(9)		

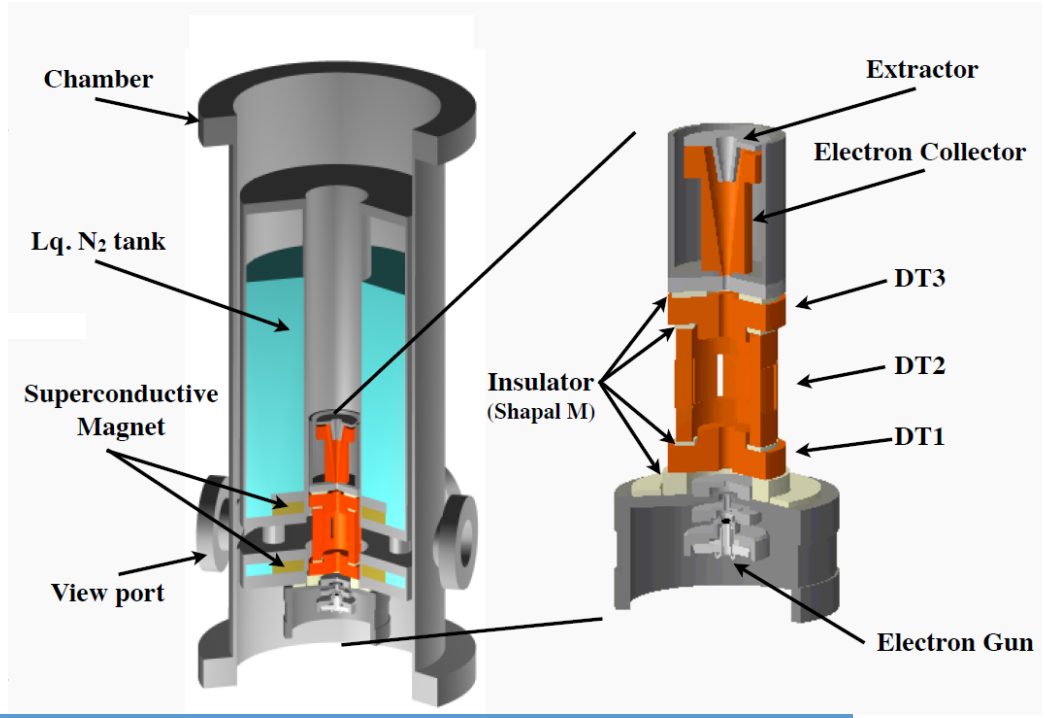
3.2 Collisional-radiative model with recombining processes for W^{27+} ion

Murakami et al. (2017) accepted in EPJD (ICAMDATA proceedings).

- Recombining processes are included for a collisional-radiative model of W^{27+} ion.
- Atomic data are calculated with HULLAC code.
- 226 Electron configurations are considered: **$4d^{10}$ 4f**, $4d^{10}$ *nl* (*n*=5-9, *l*=0-5), $4d^9 4f^2$, $4d^9$ 4f*nl* (*n*=5-9, *l*=0-5), $4d^9 5ln'l'$ (*n*=5-8, *l*,*l'*=0-5), $4d^9 6lnl'$ (*n*=6-7, *l*,*l'*=0-4), $4p^5 4d^{10} 4f^2$, $4p^5 4d^{10} 4fnl$ (*n*=5-6, *l*=0-5). In total 25,632 J-resolved levels are considered in the model.



3.4 Collaboration with Univ. Electro-Communications using Compact EBIT (CoBIT)

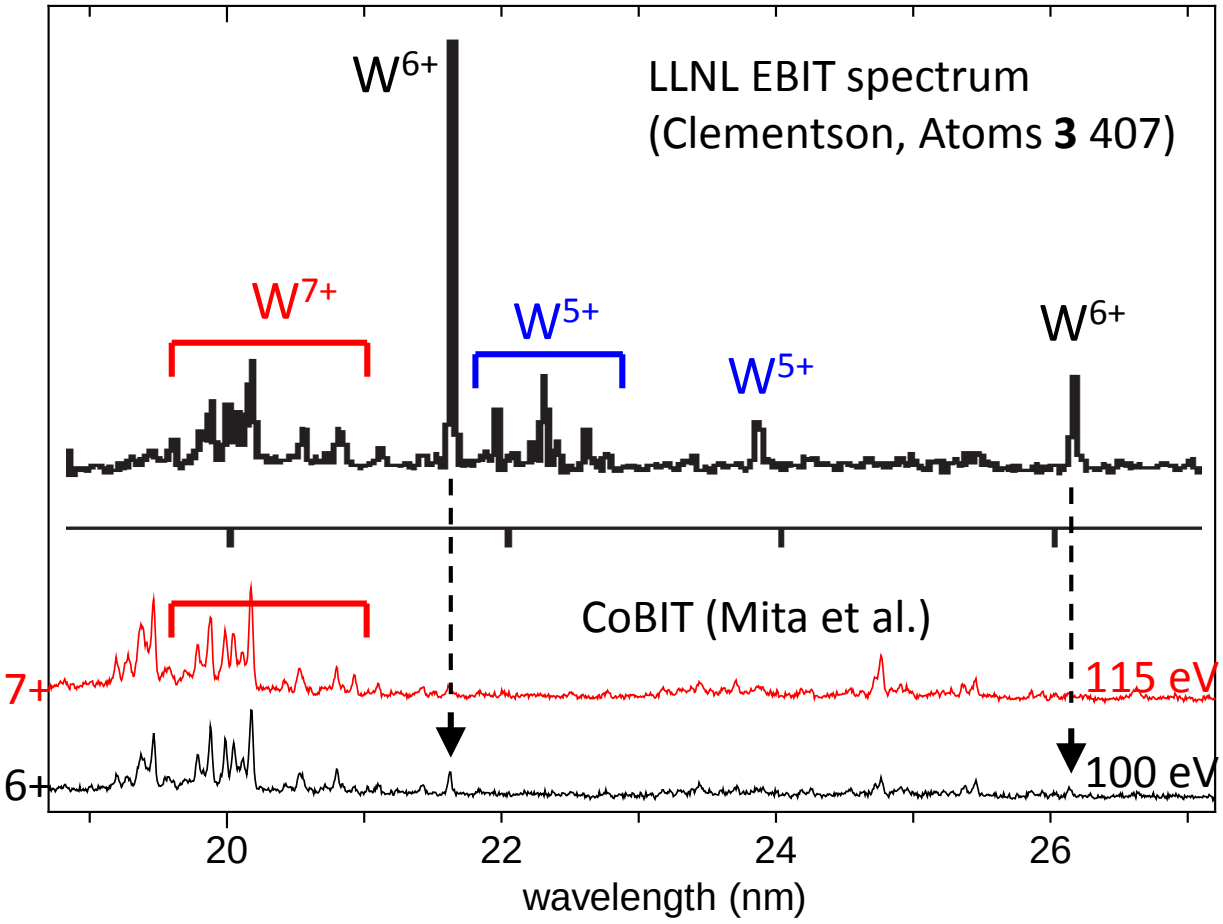


e-beam energy 100 - 2500 eV
e-beam current 20 mA (max)
B-field 0.2 T (max) @77 K (High-Tc SCM)

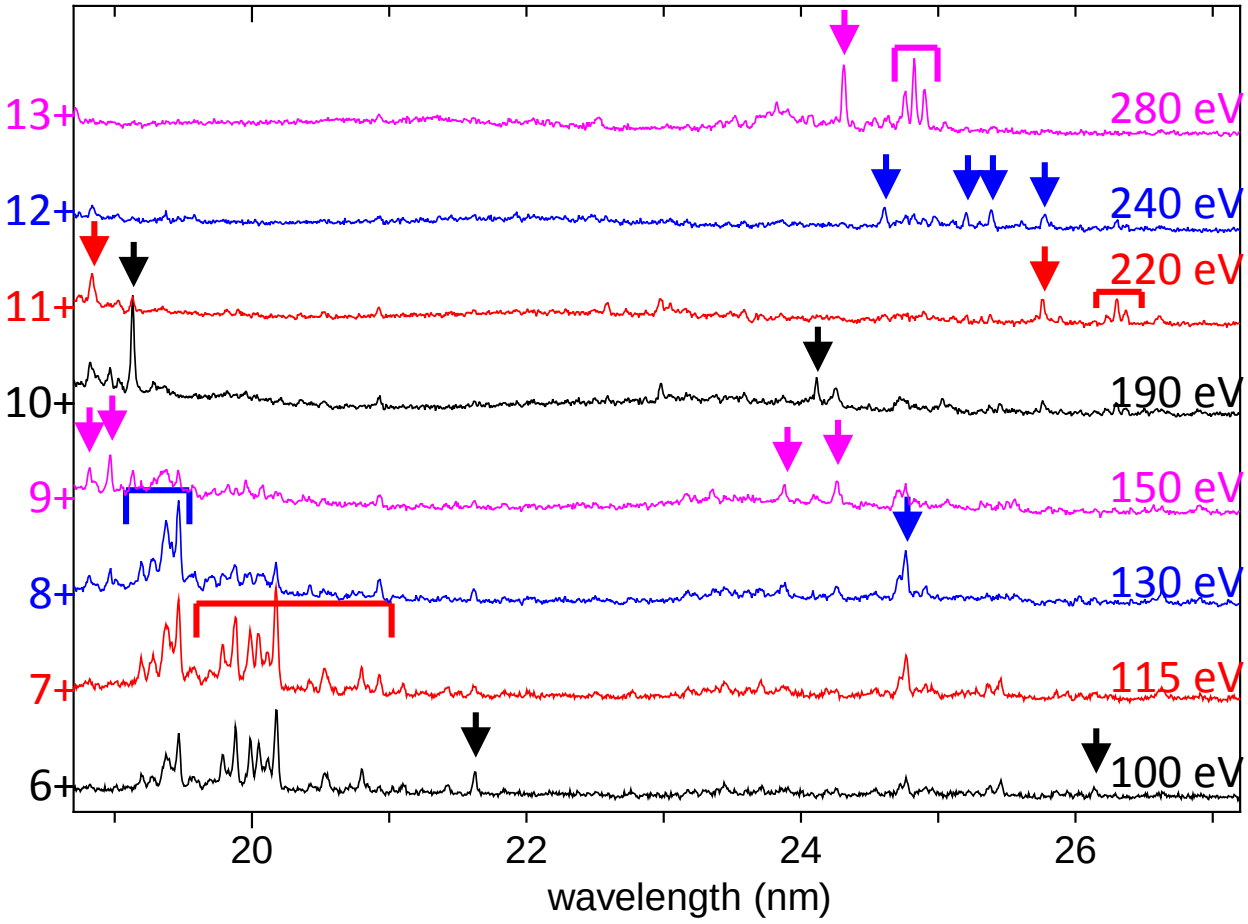
W^{q+} (q~5-30)

W EUV spectra: e-beam energy dependence

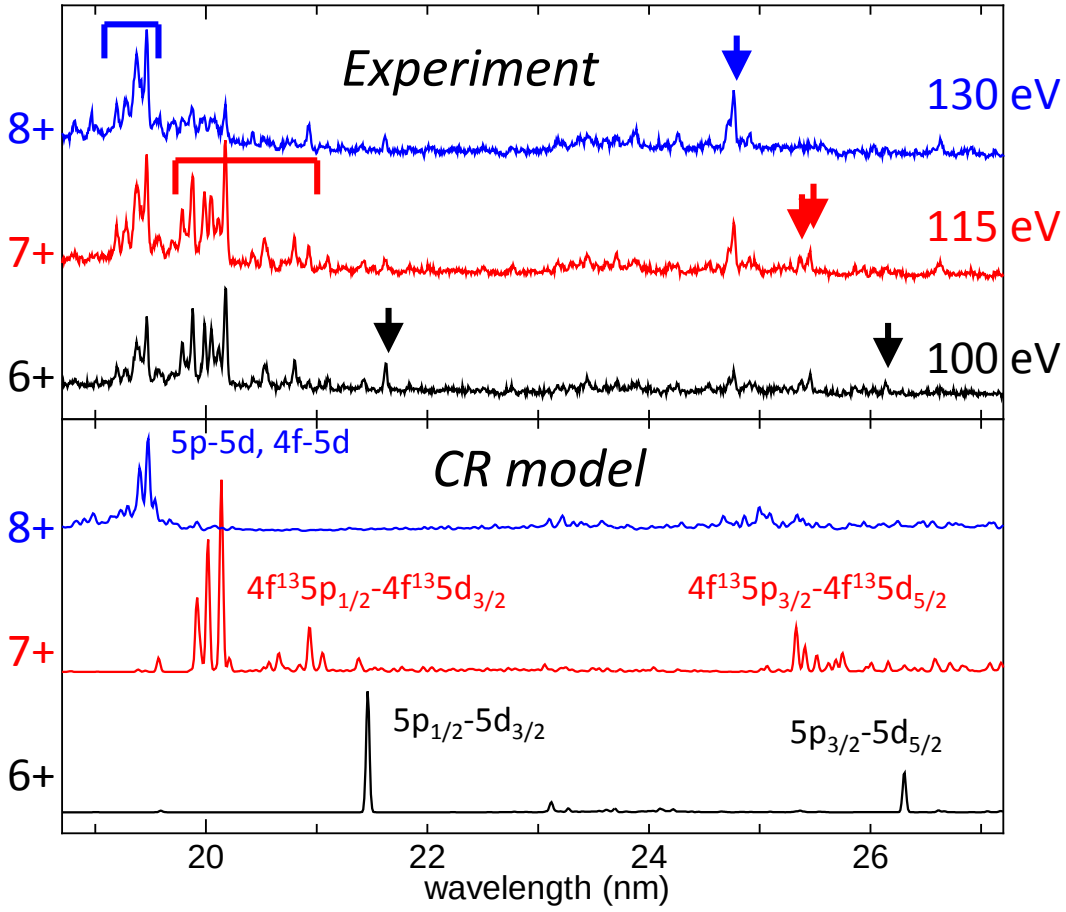
N. Nakamura (Univ. Electro-Comm.), ICPEAC XXX 2017

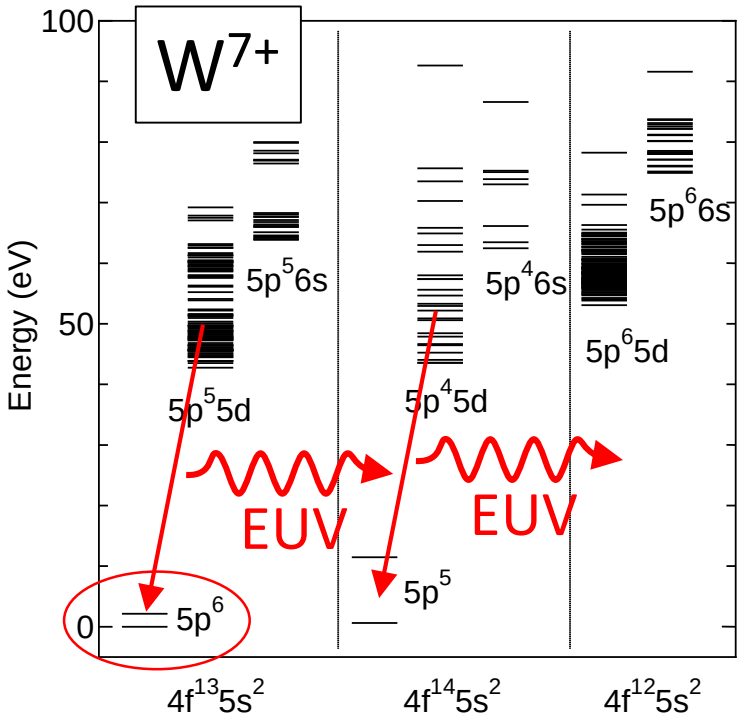


EUV spectra: e-beam energy dependence



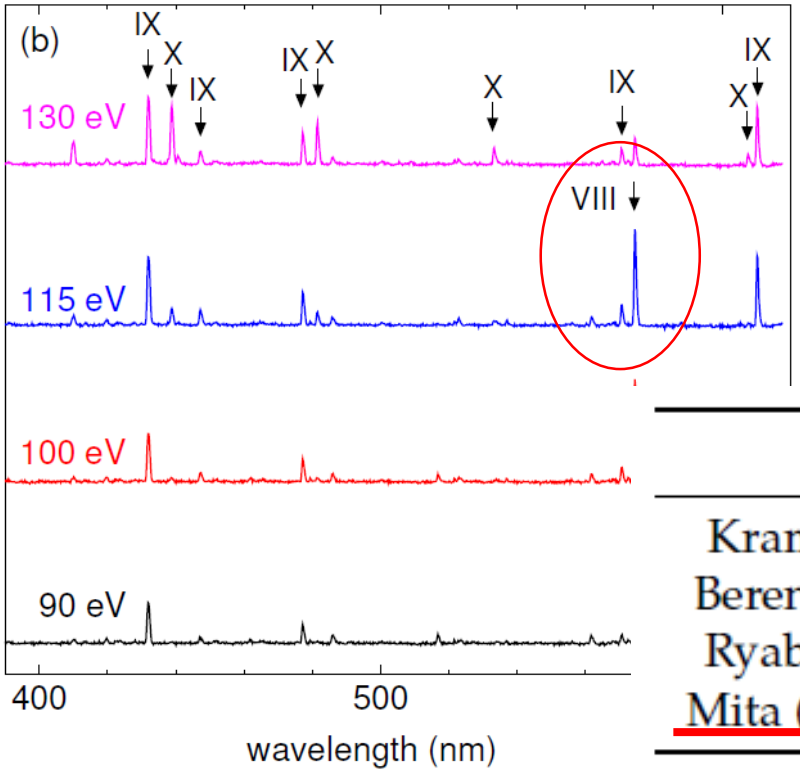
EUV spectra: comparison with CRM





Benchmarking atomic structure calculations

M1 transitions between FS splitting in the ground state configuration of W^{7+}



W^{7+} ($4f^{13}5s^25p^6$) ^2F

5/2 visible

7/2

M. Mita et al., Atoms 5 (2017) 13

	year	exp or th	energy (cm^{-1})
Kramida [5]	2009	theory	17440 ± 60
Berengut [14]	2009	theory	18199
Ryabtsev [6]	2015	experiment	17410 ± 5
Mita (present)	2016	experiment	17402.5 ± 0.9

EUV spectrum of Tm ions

C. Suzuki, F. Koike, et al. PPCF 59 (2017) 014009

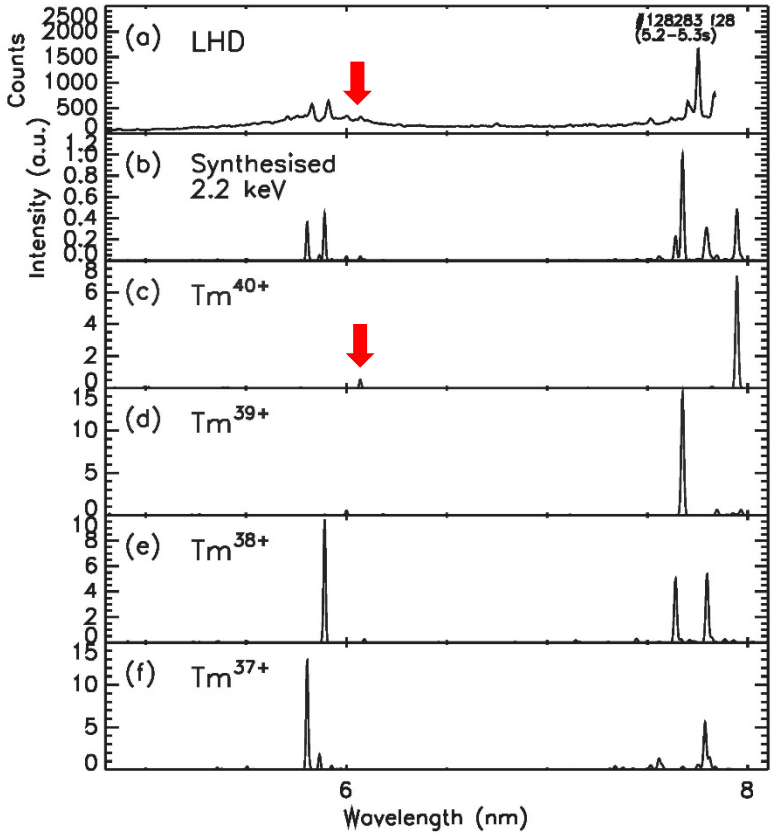


Table 1. List of the isolated lines identified experimentally for the first time in the LHD.

Ion	Transition	Wavelength (nm)	References
Ni-like			
Nd^{32+}	$3d_{3/2}4p_{1/2}$–$3d_{3/2}4d_{3/2}$	7.413	[25]
Cu-like			
Tb^{36+}	$3d^{10}4p\ ^2P_{1/2}$–$3d^{10}4d\ ^2D_{3/2}$	7.203	[26]
Tb^{36+}	$3d^{10}4d\ ^2D_{3/2}$–$3d^{10}4f\ ^2F_{5/2}$	8.796	[26]
Ho^{38+}	$3d^{10}4p\ ^2P_{1/2}$–$3d^{10}4d\ ^2D_{3/2}$	6.614	
Tm^{40+}	$3d^{10}4p\ ^2P_{1/2}$–$3d^{10}4d\ ^2D_{3/2}$	6.072	
Ag-like			
Tm^{22+}	$4d^{10}4f\ ^2F_{7/2}$–$4d^94f^2\ ^2G_{9/2}$	5.933	
Tm^{22+}	$4d^{10}4f\ ^2F_{5/2}$–$4d^94f^2\ ^2G_{7/2}$	5.986	

Note:The uncertainty of the wavelengths measured in the LHD is estimated to be less than ±0.005 nm. The details of the lines from Ho and Tm ions will be reported soon in a separate paper.

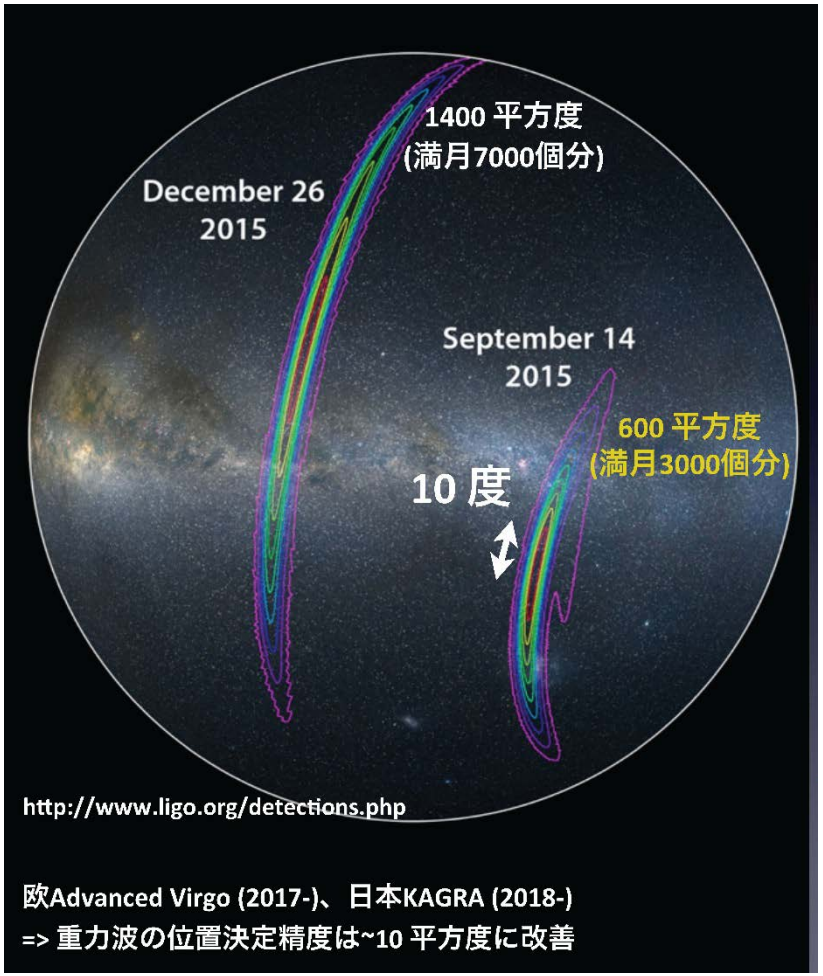
Figure 10. Comparison between the measured and modelled spectra from Tm ions at a temperature of 2.2 keV: (a) spectrum measured in LHD, (b) synthesised spectrum with assuming the abundance ratio of 0.625:1.0:1.521:1.5 for Tm^{37+}:Tm^{38-}:Tm^{39+}:Tm^{40+} and (c)–(f) calculated spectra for each ion.

- Emission lines of Tm ions measured in LHD plasma are newly identified and compared with synthesized spectrum of CR model.

3.6 New collaboration on atomic structure and opacity calculations for low-charged high-Z elements for neutron star merger.

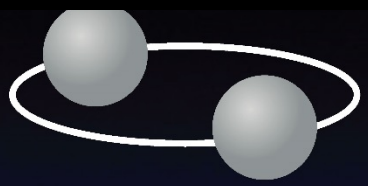
M. Tanaka (NAOJ), D. Kato (NIFS). G.Gaigalas (Vernius Univ.), et al., submitted to Ap.J (2017)

- Neutron star merger is expected to emit “gravitational wave”.
- Spatial resolution of measurements for gravitational wave is about 1400 degree^2 => too wide to identify the object.
- Identification by light curve is important to search for a source of gravitational wave.
- Opacity data are required to calculate light curve from “kilonovae” as a result of neutron star merger.



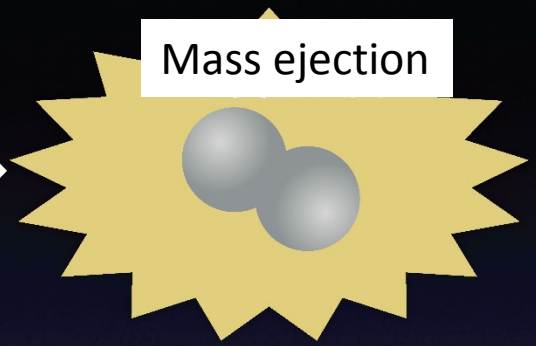
Neutron star merger → nucleosynthesis of heavy elements

Neutron star
Radius = 10km
Mass = 1.5 solar mass



< 1秒

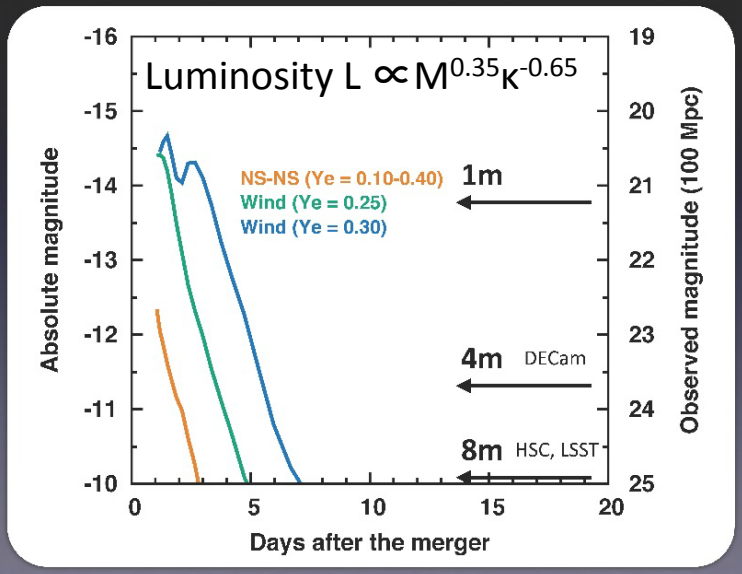
Mass ejection

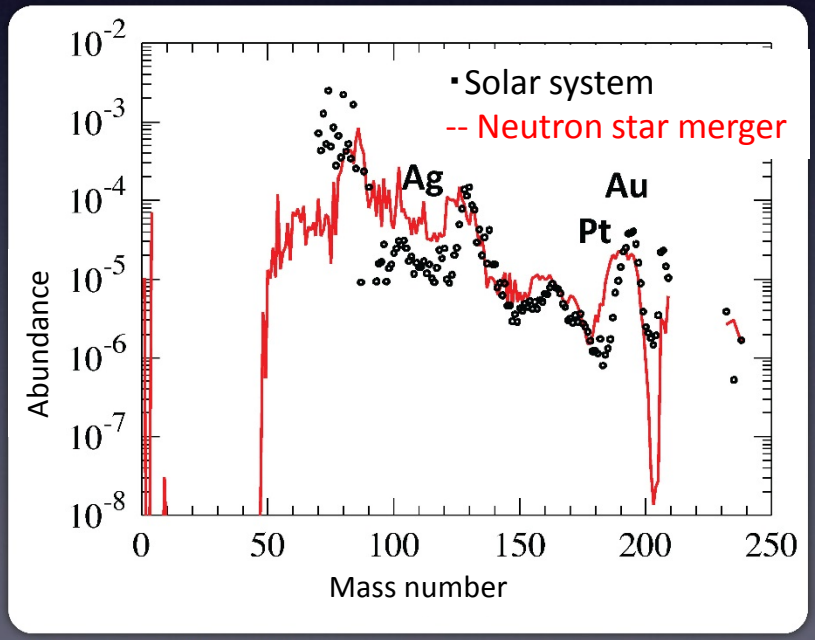


Neutron capture
(r-process)

r-band magnitude @ 100 Mpc

Mej = 0.01 Msun





Wanajo, Sekiguchi+14, ApJ, 789, L39

Atomic structure calculations

HULLAC code (relativistic, local radial potential, Bar-Shalom+99)

Se I-III (Z=34, p)

Ru I-III (Z=44, d)

Te I-III (Z=52, p)

Nd I-III (Z=60, f)

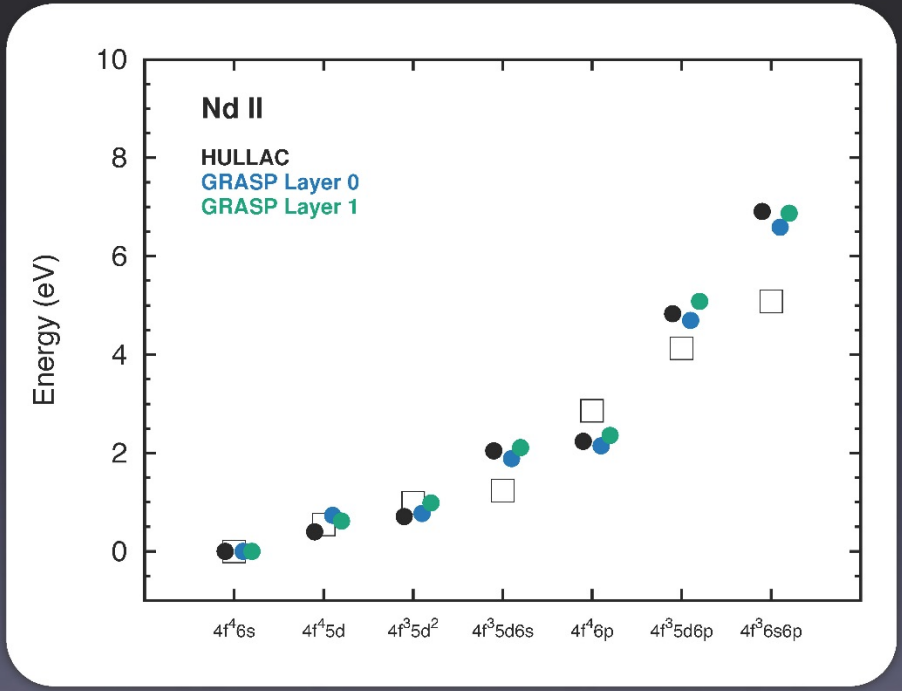
Er I-III (Z=68, f)

Ion	Configurations	Number of levels	Number of lines
HULLAC			
Se I	$\mathbf{4s^2 4p^4}$, $4s^2 4p^3(4d, 4f, 5-8l)$, $4s4p^5$, $4s4p^4(4d, 4f)$, $4s^2 4p^2(4d^2, 4d4f, 4f^2)$, $4s4p^3(4d^2, 4d4f, 4f^2)$	3076	973,168
Se II	$\mathbf{4s^2 4p^3}$, $4s^2 4p^2(4d, 4f, 5-8l)$, $4s4p^4$, $4s4p^3(4d, 4f)$, $4s^2 4p(4d^2, 4d4f, 4f^2)$, $4s4p^2(4d^2, 4d4f, 4f^2)$	2181	511,911
Se III	$\mathbf{4s^2 4p^2}$, $4s^2 4p(4d, 4f, 5-8l)$, $4s4p^3$, $4s4p^2(4d, 4f)$, $4s^2(4d^2, 4d4f, 4f^2)$, $4s4p(4d^2, 4d4f, 4f^2)$	922	92,132
Ru I	$\mathbf{4d^7 5s}$, $\mathbf{4d^6 5s^6}$, $\mathbf{4d^8}$, $4d^7(5p, 5d, 6s, 6p)$, $4d^6 5s(5p, 5d, 6s)$	1,545	250,476
Ru II	$\mathbf{4d^7}$, $4d^6(5s-5d, 6s, 6p)$	818	76,592
Ru III	$\mathbf{4d^6}$, $4d^5(5s-5d, 6s)$	728	49,066
Te I	$\mathbf{5s^2 5p^4}$, $\mathbf{5s^2 5p^3}(\mathbf{4f, 5d, 5f, 6s-6f, 7s-7d, 8s})$, $5s5p^5$	329	14,482
Te II	$\mathbf{5s^2 5p^3}$, $\mathbf{5s^2 5p^2}(\mathbf{4f, 5d, 5f, 6s-6f, 7s-7d, 8s})$, $5s5p^4$	253	9,167
Te III	$\mathbf{5s^2 5p^2}$, $\mathbf{5s^2 5p}(\mathbf{5d, 6s-6d, 7s})$, $5s5p^3$	57	419
Nd I	$\mathbf{4f^4 6s^2}$, $\mathbf{4f^4 6s}(\mathbf{5d, 6p, 7s})$, $\mathbf{4f^4 5d^2}$, $\mathbf{4f^4 5d6p}$, $4f^3 5d6s^2$, $4f^3 5d^2(6s, 6p)$, $4f^3 5d6s6p$	31,358	70,366,259
Nd II	$\mathbf{4f^4 6s}$, $\mathbf{4f^4 5d}$, $4f^4 6p$, $4f^3 6s(5d, 6p)$, $4f^3 5d^2$, $4f^3 5d6p$	6,888	3,951,882
Nd III	$\mathbf{4f^4}$, $4f^3(5d, 6s, 6p)$, $4f^2 5d^2$, $4f^2 5d(6s, 6p)$, $4f^2 6s6p$	2252	458,161
Er I	$\mathbf{4f^{12} 6s^2}$, $\mathbf{4f^{12} 6s}(\mathbf{5d, 6p, 6d, 7s, 8s})$, $4f^{11} 6s^2(5d, 6p)$, $4f^{11} 5d^2 6s$, $4f^{11} 5d6s(6p, 7s)$	10,535	9,247,777
Er II	$\mathbf{4f^{12} 6s}$, $4f^{12}(5d, 6p)$, $4f^{11} 6s^2$, $4f^{11} 6s(5d, 6p)$, $4f^{11} 5d^2$, $4f^{11} 5d6p$	5,333	2,432,665
Er III	$\mathbf{4f^{12}}$, $4f^{11}(5d, 6s, 6p)$	723	42,671

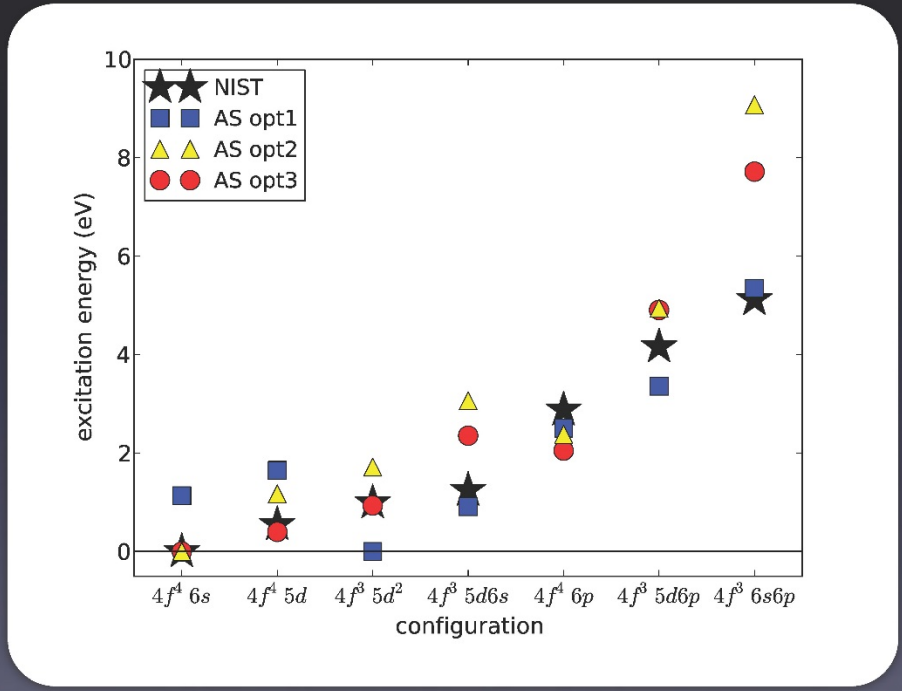
GRASP2K code (relativistic, e-e correlation, Jonsson+07)

Nd II-III, Er II-III

Energy levels of Nd II



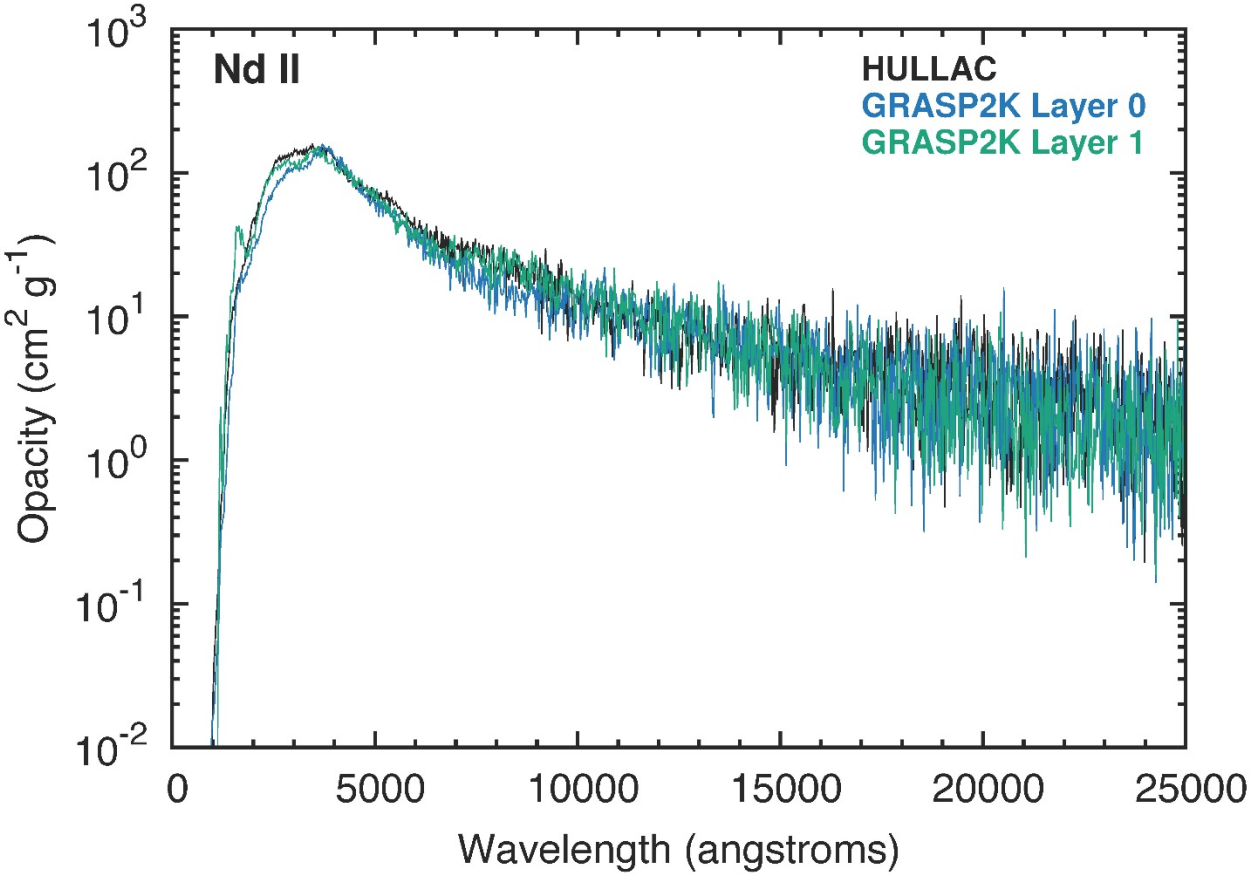
MT+ in prep



Kasen+13 (Autostructure code)

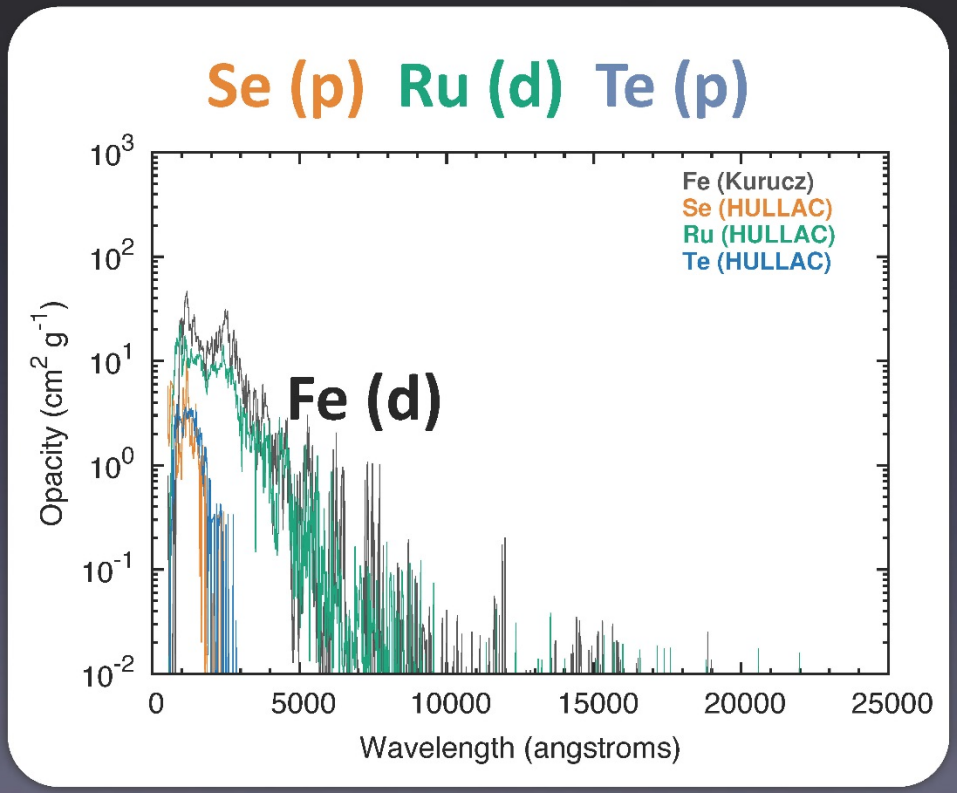
Line expansion opacity of Nd II

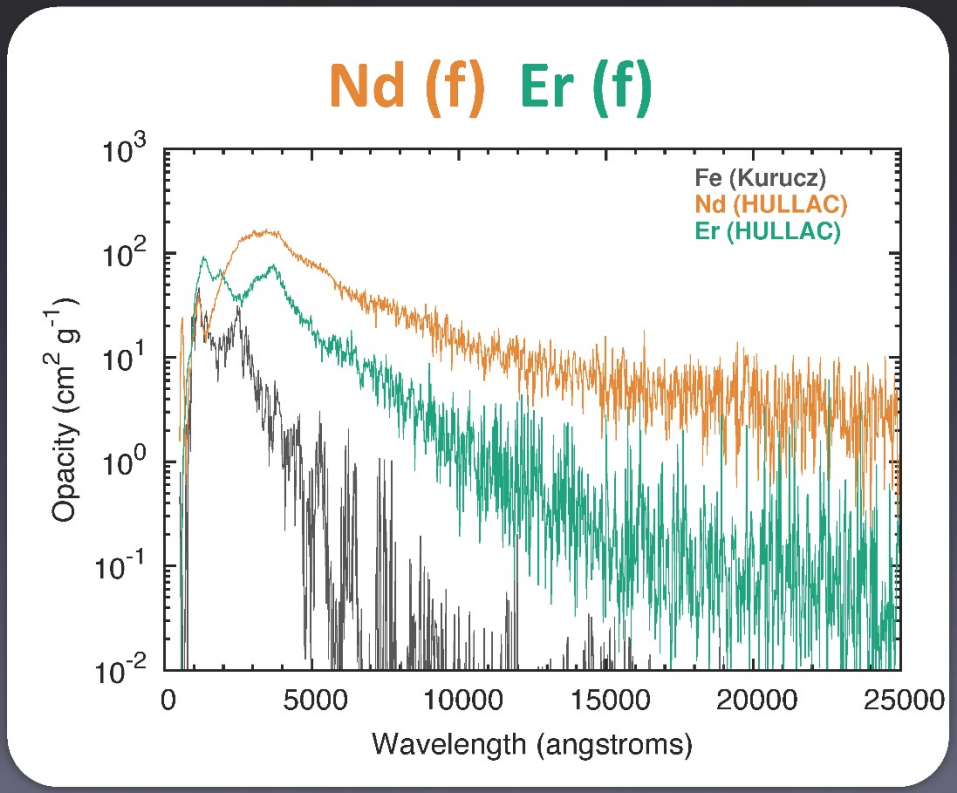
T = 5,000 K, ρ = 10^{-13} g cm^{-3}, t = 1 day



Opacities from two codes agree very well

Line expansion opacity (for each element)





MT+ in prep.

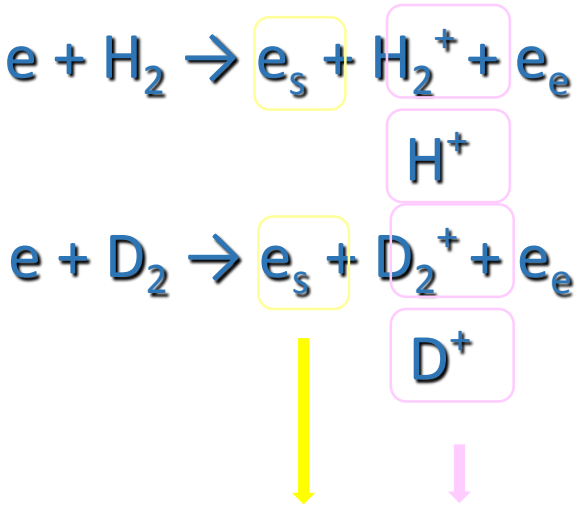
κ (p shell) << κ (d shell) << κ (f shell)

see Kasen+13, Fontes+17

3.7 Isotope effect in dissociation processes of deuterated molecules from doubly excited states

Y. Sakai (Toho Univ.) et al., AMPP2016 in Chengdu, China
NIFS-PROC-103 (2017), p.26

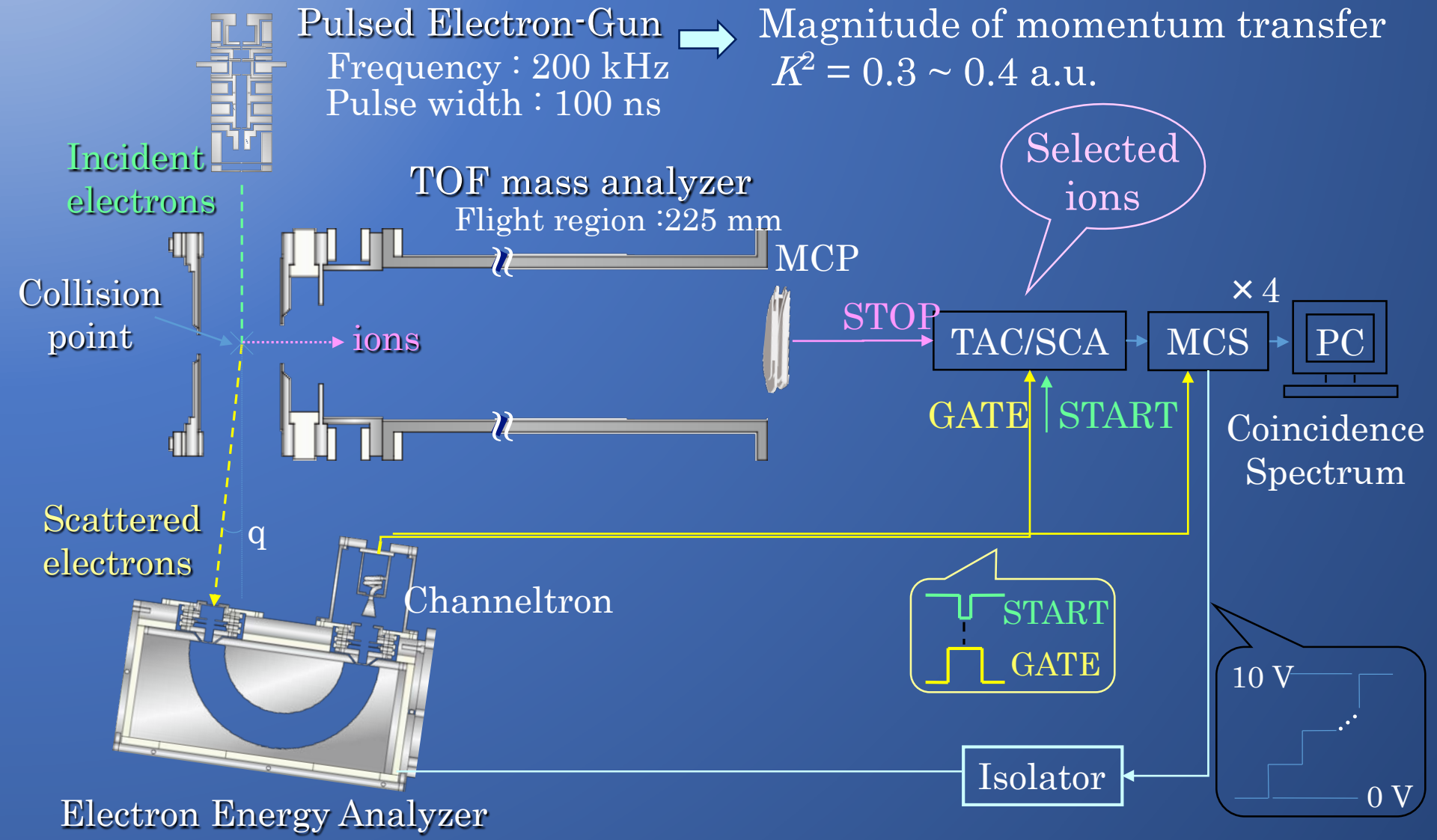
- Generalized oscillator strength distribution (GOSDs) for ionization of H_2 and D_2 were measured by electron energy-loss spectra of scattered electron and ion coincidence measurements.



Scattered electron – ion coincidence (SEICO) measurements

Experimental Conditions

Incident electron energy : 200 eV
Electron scattering angle : 6 degree



Determination of absolute DDCS and GOSD

Mixed gas method

Electron energy-loss spectra of D_2-He mixture and D_2 (200 eV, 6 deg)

Absolute differential cross section for x : $(d\sigma/d\Omega)_x$

$$\left(\frac{d\sigma}{d\Omega}\right)_x = \frac{I_x}{I_{2^1P}}\left(\frac{d\sigma}{d\Omega}\right)_{2^1P} \times C$$

I : Inteisnty

$\left(\frac{d\sigma}{d\Omega}\right)_{2^1P}$: DCS of He 2^1P state [9]

C : Correlation term
From mixing ratio and number density

[9] T. Y. Suzuki *et al. Phys. Rev. A*, **57**, 1832 (1998).

4. Concluding remarks

- A&M database activities:
  - The server is replaced in 2016 and the database system is running with PostgreSQL.
  - Implementation to VAMDC is still pending.
- A & M data related activities:
  - LHD experimental group on AM processes continues to measure various spectra of W and high Z ions and activate our AM related research.
  -Domestic collaboration projects are progressed.
- No NIFS-DATA publication since 2014.