

# NIFSにおける原子分子データ 活動

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# 活動内容

- NIFS一般共同研究
  - 原子分子データ収集作業会
  - 新しいデータベースシステムの開発(データベース活動支援ツール)
- 他分野との連携
  - 太陽上層大気診断のための鉄イオン原子過程データ(国立天文台, 電気通信大学)
  - 放電基礎パラメータ(電気学会調査専門委員会)
  - 原子分子データベース協会
- IAEA DCN&CRPへの参加

## 最近のDBアップデートから

核融合研 共同研究 平成18年度－  
「LHDの周辺プラズマのための高Z原子及び分子の原子分子  
データベース作成」  
(代表:北島昌史 東工大)

Ar, Fe, Ni, Kr, Mo, Xe, Wなどの電子衝突および重粒子  
衝突断面積. 同位体や $\text{H}_3^+$ を含む水素分子の電子衝突断  
面積. (活動報告をNIFS-DATAに投稿準備中)

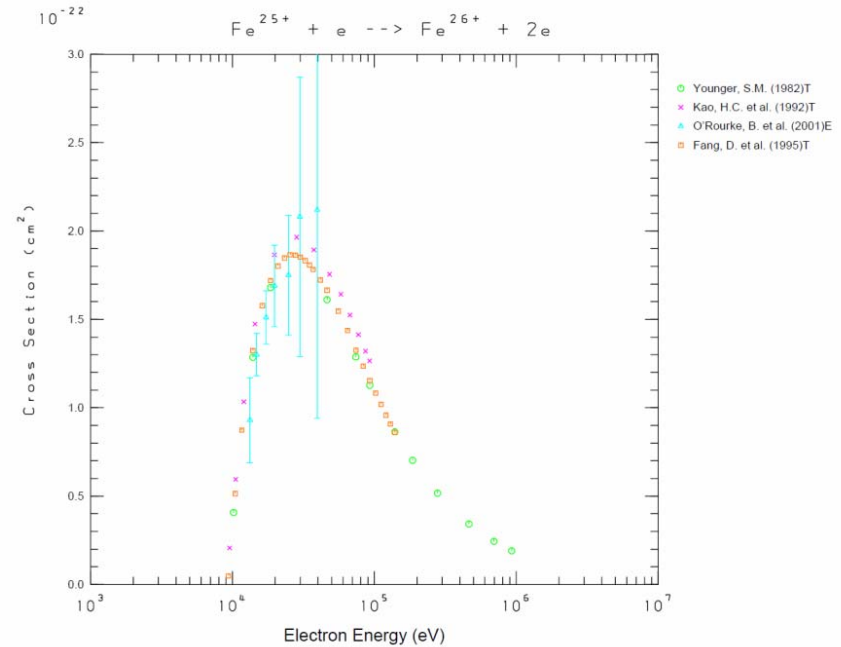
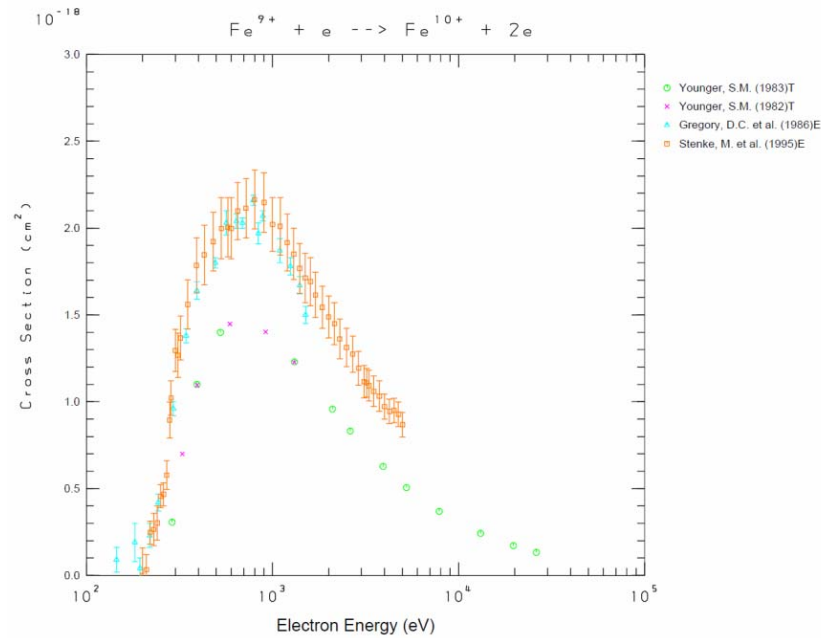
# Working Group for NIFS A&M Data Collection

- Members
  - M. Kimura (Kyushu Univ.)
  - T. Kusakabe (Kinki Univ)
  - M. Imai (Kyoto Univ.)
  - K. Motohashi (TUAT)
  - A. Igarashi (Miyazaki Univ)
  - T. Morishita (UEC)
  - K. Moribayashi (JAEA)
  - L. Pichl (ICU)
  - H. Suno (JAMSTEC)
  - K. Okuno (TMU)
  - K. Soejima (Nigata Univ.)
  - K. Ishii (Nara Wemen's Univ.)
  - M. Hoshino (Sophia Univ.)
  - A. Watanabe (Ochanomizu WU)
  - M. Kitajima (Tokyo Inst. Tech.)
  - H. Sakaue, D. Kato, M. Goto, S. Morita, K. Sato, H. Funaba, T. Ido, B. Peterson (NIFS)

# 2007年度の成果

- データ収集
  - Fe, Ni, Mo, W, Ne, Ar, Kr, Xe
    - これらの元素(原子、イオン)と原子分子との衝突過程の断面積
    - これらの元素(原子、イオン)による電子衝突過程の断面積
      - 例; W; AMDIS-3件、0(E), +42(T), +70(T)
      - 例; Fe; AMDIS-52件
        - » Ionization: 4, +0(E), +21(T), +24(T), +25(E)
        - » Recombination: 12, +16(2T), +17(3T), +18(5T), +19(3T), +20(3T), +21(3T), +22(3T), +23(3T), +24(2T), +25(T)
        - » Excitation: 36, +1(T), +2(T), +3(T), +4(T), +8(T), +9(2T), +10(T), +11(T), +12(2T), +14(3T), +16(3T,E), +17(T), +18(3T), +19(3T), +20(5T), +21(5T), +22(5T), +23(6T), +24(2T), +25(T)
    - 実験的研究によるデータは3件のみ
  - Report on Cross Section Data Compilation for Electron and Ion Collisions with High Z Elements (M. Kitajima et al., NIFS-DATA, *in preparation*)

# AMDIS; e-Feデータの一例



- 実験と理論の一致が良い場合と悪い場合が顕著
  - － 実験: イオンビームのコンタミネーション(準安定状態etc)
  - － 理論: 取り込む過程(EAなど)の不足
- 引き続きデータ収集が必要

# 光吸収過程データに関する検討

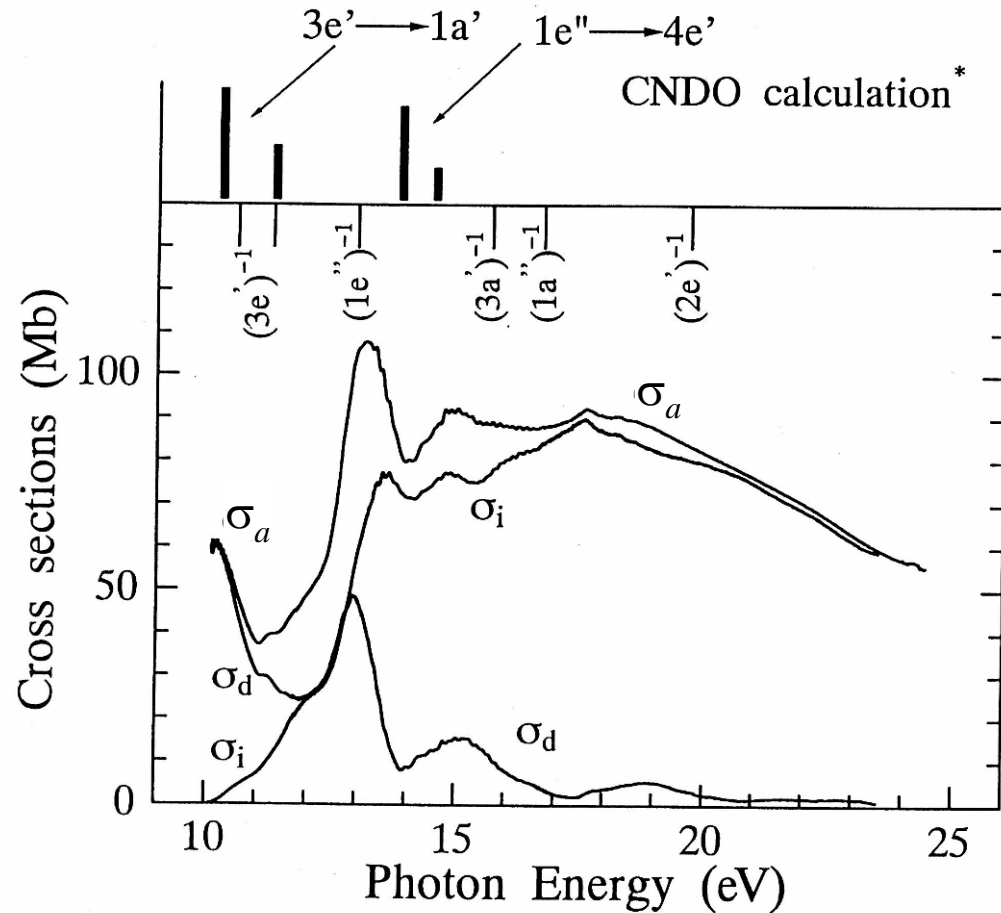
- 光吸収過程データに関する検討
  - 核融合プラズマを強い放射光源とした周辺部で光吸収過程の評価に必要な
- いくつかのデータ例
  - 炭化水素
    - Evaluated data
      - List of molecules
      - diatomic molecules:  $H_2$ ,  $N_2$ ,  $O_2$ ,  $Cl_2$ ,  $CO$ ,  $NO$ ,  $HF$ , and  $HCl$
      - triatomic and relatively simple molecules:  $H_2O$ ,  $CO_2$ ,  $H_2S$ ,  $N_2O$ ,  $CS_2$ ,  $OCS$ ,  $SO_2$ ,  $NH_3$ , and  $SF_6$
      - silanes:  $SiH_4$  and  $Si_2H_6$
      - hydrocarbons:  $CH_4$ ,  $C_2H_6$ ,  $C_2H_4$ ,  $C_2H_2$ ,  $C_3H_4$ ,  $cyclo-C_3H_6$ ,  $C_3H_8$ , and  $C_6H_6$
      - halocarbons:  $CF_4$  and  $CCl_4$
      - alcohols and ethers:  $CH_3OH$ ,  $CH_3OCH_3$ , and  $CH_3OC_2H_5$

K. Kameta, N. Kouchi, and Y. Hatano, *Landolt–Bornstein Numerical Data and Functional Relationships in Science and Technology*, ed. by W. Martienssen, New Series, Group 1, Vol. 17, Pt C ~Springer, Tokyo, 2003.

# 炭化水素の光吸収断面積の例

Cyclo-propane

- $\sigma_a$ : 光吸収断面積
- $\sigma_i$ : 光イオン化断面積
- $\sigma_d$ : 中性解離断面積
- $\sigma_a$  に多くの構造
- $\sigma_a : \sim 10^{-16} \text{cm}^2$
- $\sigma_a > \sigma_i$   
below 25eV
- $\sigma_a \cong \sigma_d$   
near threshold





# Available experimental absolute cross-section data for ions

- Singly ionized atom;  
He<sup>+</sup>, B<sup>+</sup>, C<sup>+</sup>, N<sup>+</sup>, O<sup>+</sup>, Ne<sup>+</sup>, Mg<sup>+</sup>, Al<sup>+</sup>, S<sup>+</sup>, K<sup>+</sup>, Ca<sup>+</sup>, Sc<sup>+</sup>, Ti<sup>+</sup>, V<sup>+</sup>, Cr<sup>+</sup>,  
Mn<sup>+</sup>, Fe<sup>+</sup>, Co<sup>+</sup>, Ni<sup>+</sup>, Zn<sup>+</sup>, Ga<sup>+</sup>, Sr<sup>+</sup>, I<sup>+</sup>, Xe<sup>+</sup>, Cs<sup>+</sup>, Ba<sup>+</sup>, La<sup>+</sup>
- Doubly ionized atom;  
C<sup>2+</sup>, N<sup>2+</sup>, O<sup>2+</sup>, F<sup>2+</sup>, Al<sup>2+</sup>, Si<sup>2+</sup>, Ca<sup>2+</sup>, Sc<sup>2+</sup>, I<sup>2+</sup>, Xe<sup>2+</sup>, Ba<sup>2+</sup>
- Highly charged atomic ions;  
N<sup>3+</sup>, O<sup>3+</sup>, O<sup>4+</sup>, F<sup>3+</sup>, F<sup>4+</sup>, Ne<sup>3+</sup>, Ne<sup>4+</sup>, Ti<sup>3+</sup>, Fe<sup>4+</sup>, Xe<sup>3+</sup>, Xe<sup>4+</sup>, Xe<sup>5+</sup>,  
Xe<sup>6+</sup>, Ba<sup>3+</sup>, La<sup>3+</sup>, Ce<sup>4+</sup>
- Negative ions  
He<sup>-</sup>, Li<sup>-</sup>, B<sup>-</sup>, C<sup>-</sup> (Relative), Na<sup>-</sup>, S<sup>-</sup>, Cl<sup>-</sup>, V<sup>-</sup>, Cr<sup>-</sup>, Co<sup>-</sup>, Ni<sup>-</sup>, Te<sup>-</sup>,  
I<sup>-</sup>

H. Kjeldsen, J. Phys. B. **39**, R325 (2006)

# 今後の展望

- データベース維持
  - 継続的である必要;方法
  - データベースの信頼性;ユーザーの使い勝手
    - 信用出来ないデータはデータベースには入れていない
- 不足データ
  - H<sub>2</sub> ;核融合研究に重要、データ収集計画を策定(2008年度に実施)
- 核融合研究に不足しているデータ
  - 光学的データについて
    - 既存のデータ集、データベースの調査
    - NIFS原子分子データベースとして扱えるか(扱うべきか)検討
  - 微分断面積データについて
    - プラズマ解析、シミュレーションには有用
      - データベースの再構築が必要

# Other database developed by domestic collaboration

Numerical and graphical databases for  
Differential Cross Sections of Ionization for  
Atomic Hydrogen by Proton Impact (L. Pichl,  
Japan)

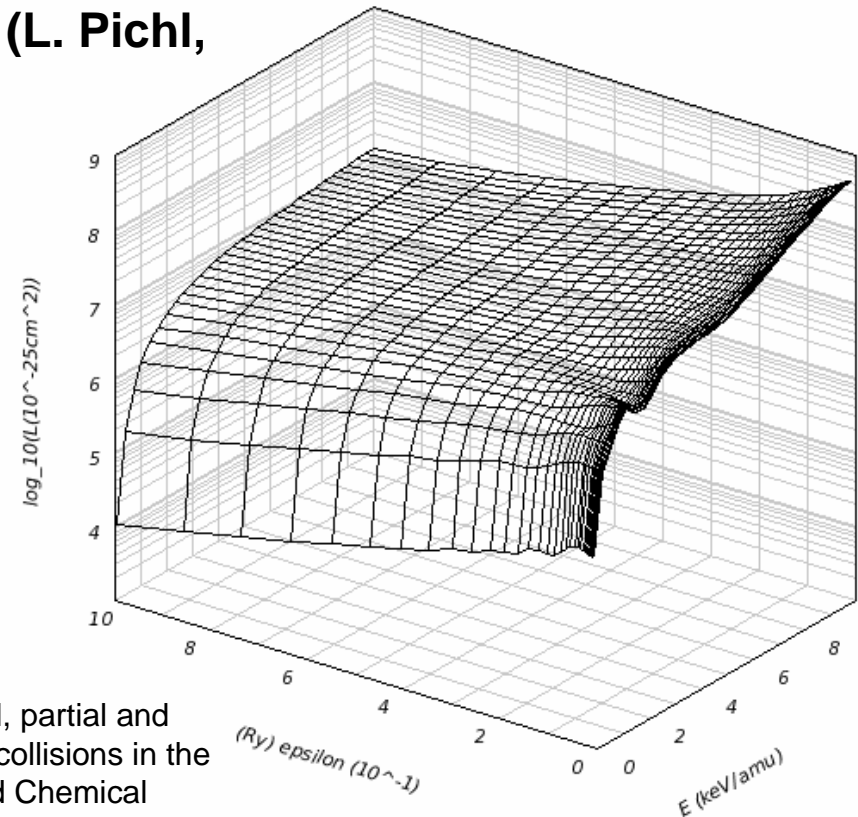
<http://crdb.nifs.ac.jp/dcsdb/>

$p\pi$    $d\pi$   
  $f\pi$    $g\pi$    $h\pi$   
  $f\sigma$    $g\sigma$    $h\sigma$   
  $s\sigma$    $p\sigma$    $d\sigma$

angle 70  
Z-min 4  
Z-grad 6

reset

search



## References:

- 1) L. Pichl, S. Zou, M. Kimura, I. Murakami, and T. Kato, Total, partial and differential ionization cross sections in proton-hydrogen atom collisions in the energy region of 0.1 keV/u - 10keV/u, Journal of Physical and Chemical Reference Data, Vol.33(2004) 1031-1058.
- 2) S. Zou, L. Pichl, M. Kimura and T. Kato, Total and differential cross section calculations for proton-impact ionization of hydrogen at low energies, Physical Review A, Vol.66 (2002) 042707:1-13.

## 最近のDBアップデートから

M. Hoshino et al.

“Elastic differential cross sections for electron collisions with polyatomic molecules”

NIFS-DATA-101, Jan. 2008

–DCS measurements (1-100 eV) at Sophia University since 1978, Australian National University, Flinders University, and Chungnam National University.

Table 1: List of molecules tabled in this report

A. Fusion Plasma-Related Gases

CH<sub>4</sub>, C<sub>2</sub>H<sub>6</sub>, C<sub>3</sub>H<sub>8</sub>, C<sub>2</sub>H<sub>4</sub>, C<sub>3</sub>H<sub>6</sub>, *isomers*-C<sub>3</sub>H<sub>4</sub>

B. Processing Plasma-Related Gases

CF<sub>4</sub>, C<sub>2</sub>F<sub>6</sub>, C<sub>3</sub>F<sub>8</sub>, C<sub>3</sub>F<sub>6</sub>, *cyclo*-C<sub>4</sub>F<sub>8</sub>, C<sub>2</sub>F<sub>4</sub>, C<sub>6</sub>F<sub>6</sub>,

CH<sub>3</sub>F, CH<sub>2</sub>F<sub>2</sub>, CHF<sub>3</sub>

NF<sub>3</sub>, SF<sub>6</sub>

SiH<sub>4</sub>, Si<sub>2</sub>H<sub>6</sub>, GeH<sub>4</sub>

C. Environmental Issues -Related Gases

CF<sub>3</sub>Cl, CF<sub>3</sub>Br, CF<sub>3</sub>I

H<sub>2</sub>O, CO<sub>2</sub>, N<sub>2</sub>O

# データベースビルダー

http://ardbnifs.ac.jp/crsdb2/

## Differential Cross-Section Database Builder

Selected Database: db1  
Number of Labels: 4  
Dimension: 2

Table Name:

- Only alphabet (lower case), numbers, and an underscore ( `_` ) are available.
- Database name must start with *alphabet*.
- [Pre-defined words will not be accepted.](#)

label1:   
label2:   
label3:   
label4:

Choose data input method:  File Upload  Manual Typing

Number of Data:





(NOTE: [Examples of Acceptable File Formats](#))

Database: db3  
Table: table1  
Decimal Place: :0

2.20000000003.500000000  
5.30000000006.600000000

x	y	z
SELECT	SELECT	3.300000000
1	100000000	
4	400000000	

[ [Back to Previous Page](#) | [Select Another Database](#) | [crsdb2 TOE](#) ]

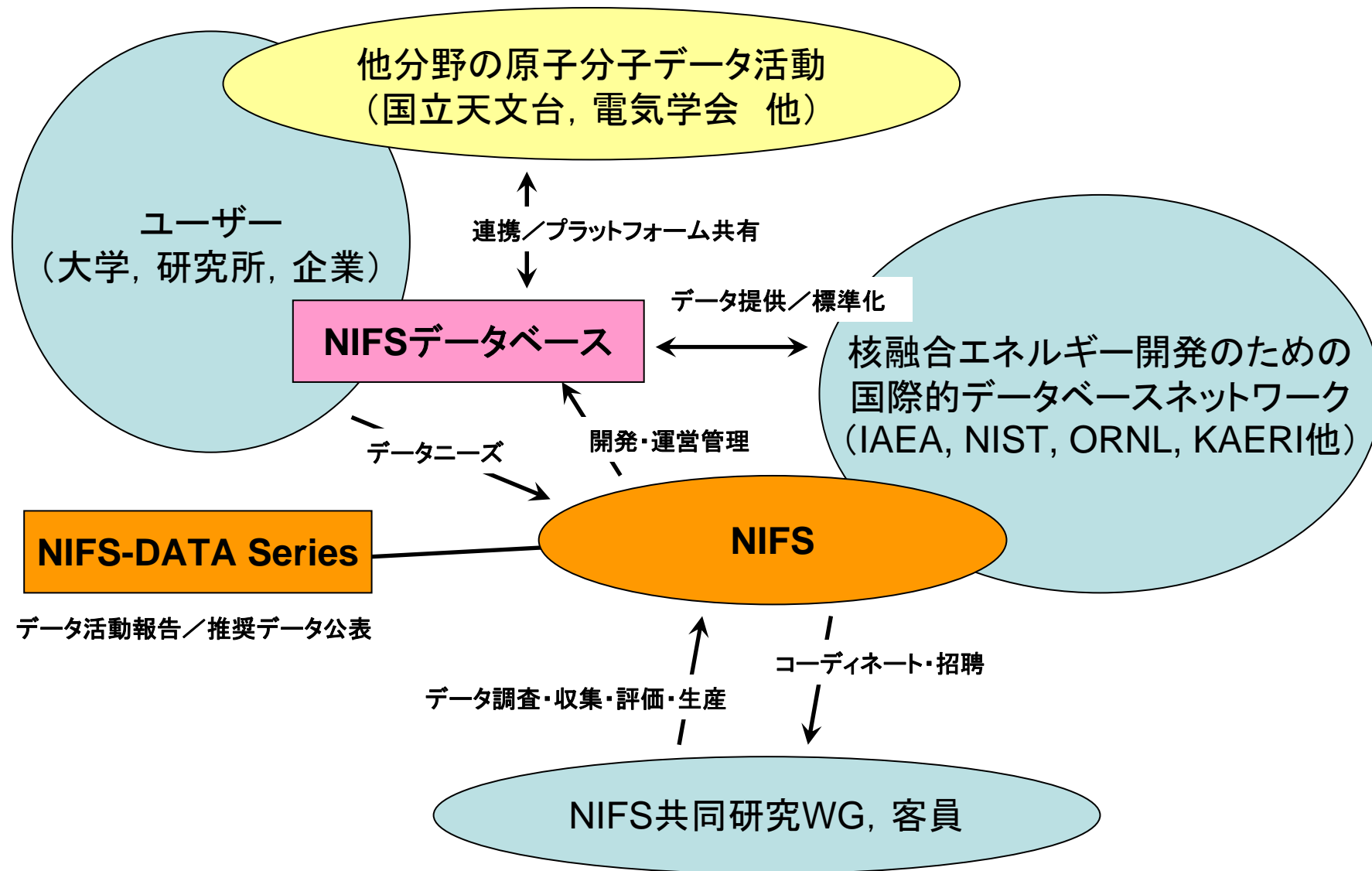
L. Pichl (ICU, Japan)

# 原子分子関連の文献情報の自動データベース化

The screenshot shows a web interface for a joint search. At the top, there is a blue banner with the ICU logo on the left, the text "Joint Search" in the center, and the NIFS logo on the right. Below the banner, the text "SPINWEB Database & IOP Electronic Journals" is displayed. The main search area contains three input fields, each preceded by an "AND" dropdown menu. To the right of each input field is the word "in" followed by a dropdown menu set to "Full Bibliographic Record". Above the second and third dropdowns is the text "Keep default or choose another field.". Below the search fields, there is a "SELECT DATABASE:" section with three checkboxes: "Both Databases", "SPINWEB", and "IOP". At the bottom of the search area are "search" and "reset" buttons. The footer of the interface features the Scitation and IOP logos, and a list of links: "[ Prof. Itikawa's list | Evolutionary Database | Bibliography Database ]".

L. Pichl, M. Suzuki, K. Joe, D. Kato, and A. Sasaki,  
“Networked database builder and data-mining engine for electronic journal papers”,  
Int. J. Comput. Sci. Eng., Vol. 2 (2006) 253-261.

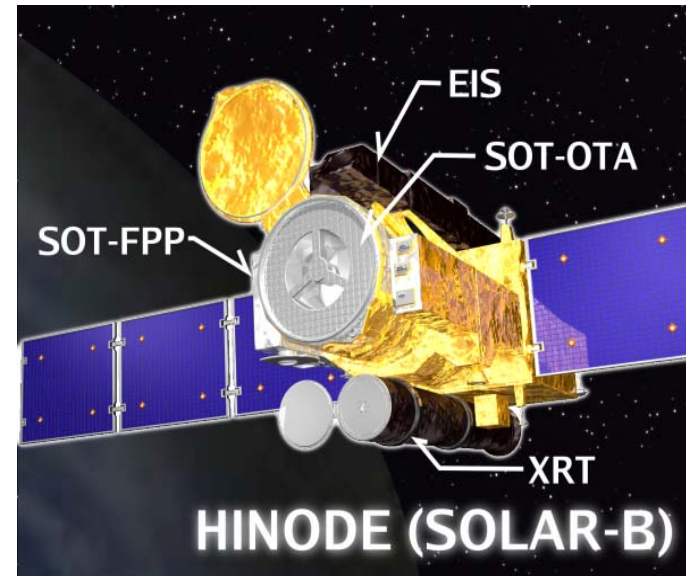
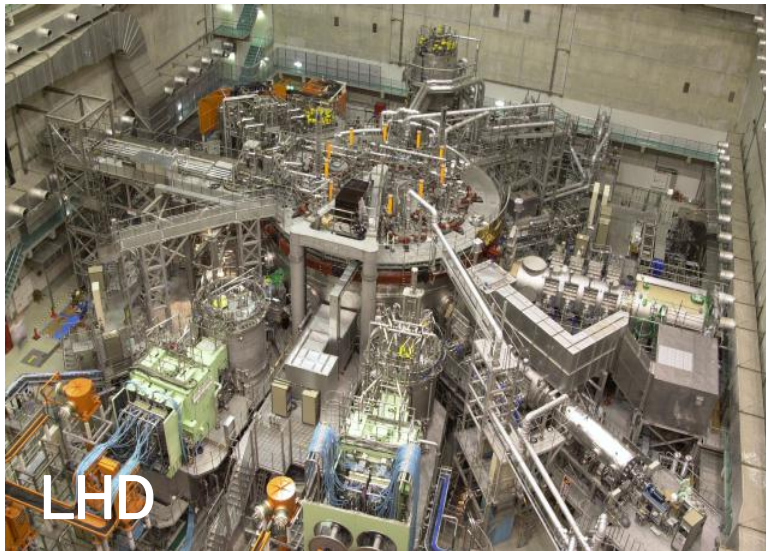
# NIFSの原子分子データベース活動ネットワーク



# Fe data for non-equilibrium ionization in LHD and Solar-atmosphere

**Hinode(Solar-B) satellite launched in September, 2006.**

X-ray and EUV telescopes would reveal heating mechanisms of active solar corona.



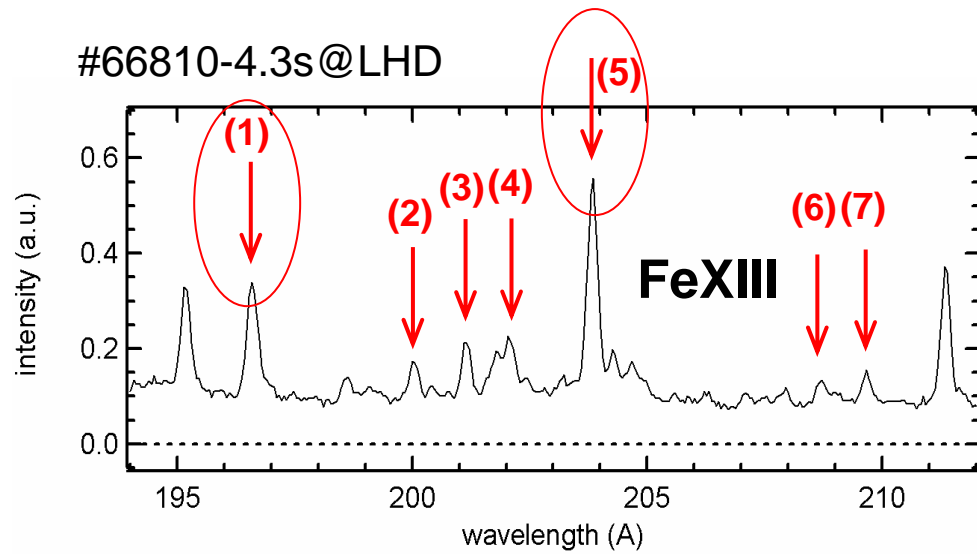
Ref. <http://solar-b.nao.ac.jp/>

## **Large Helical Device (LHD)**

EUV spectroscopy would reveal impurity transport of heavy elements in fusion plasmas.

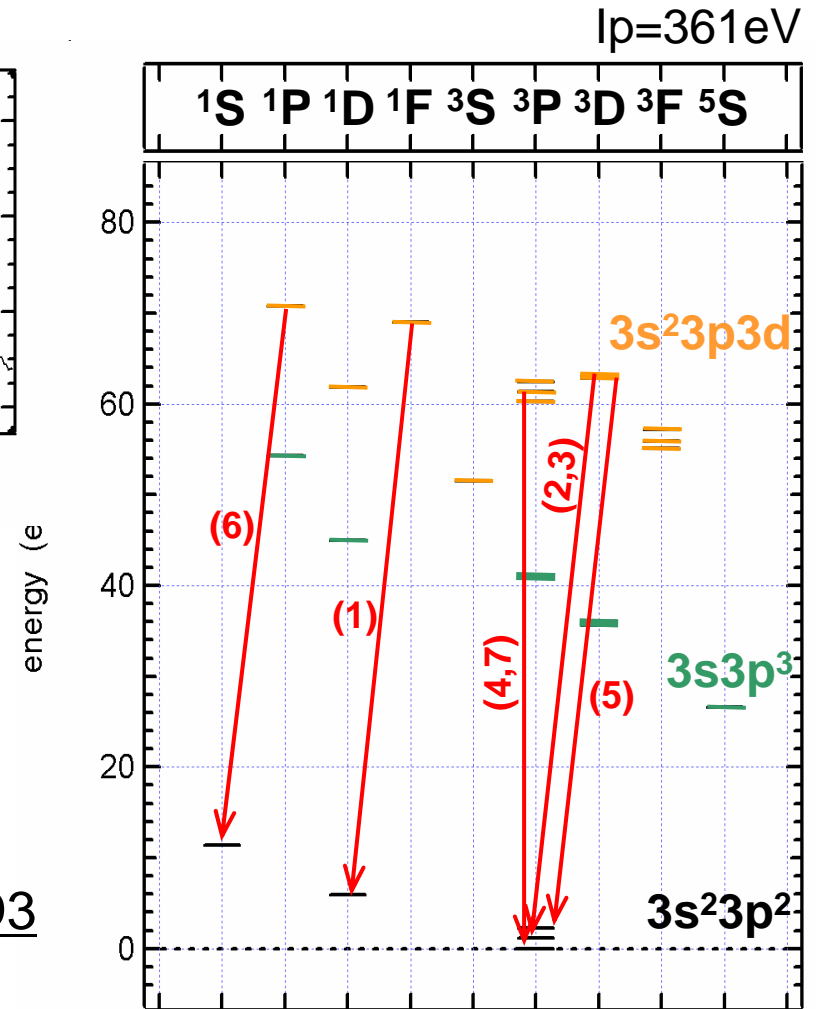


# Density diagnostics by Fe XIII lines



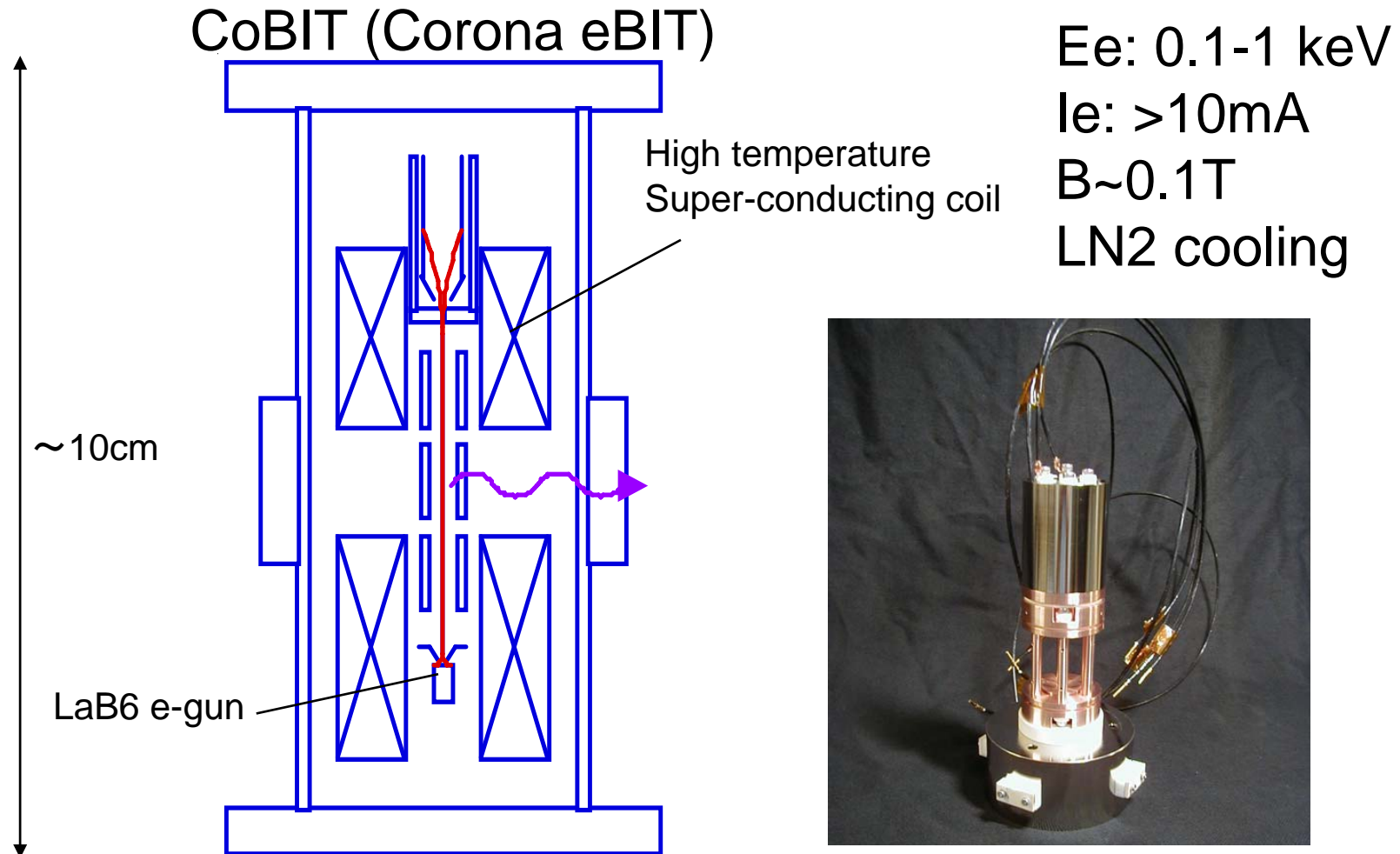
## 3p-3d transition ( $3s^23p^2-3s^23p3d$ )

- (1) **196.525Å**: 1D<sub>2</sub>-1F<sub>3</sub> (with FeXII)
- (2) **200.021Å**: 3P<sub>1</sub>-3D<sub>2</sub>
- (3) **201.121Å**: 3P<sub>1</sub>-3D<sub>1</sub> (with FeXII)
- (4) **202.044Å**: 3P<sub>0</sub>-3P<sub>1</sub>
- (5) **203.793Å+203.826Å**: 3P<sub>2</sub>-3D<sub>2,3D3</sub>
- (6) **208.679Å**: 1S<sub>0</sub>-1P<sub>1</sub>
- (7) **209.617Å**: 3P<sub>1</sub>-3P<sub>2</sub>



N. Yamamoto (Osaka Univ.)

# EUV spectroscopy of Fe ions by means of Low energy Electron-Beam-Ion-Trap



N. Nakamura (UEC) & H.A. Sakaue (NIFS)

## 電気学会のデータベース活動との連携

核融合研 共同研究

「プロセスプラズマ関連の原子・分子データベースネットワーク構築」  
平成16年度～平成18年度（代表:田中大 上智大）

プラズマプロセス、放電、大気化学  
「広い意味でのプラズマ科学への活用」

電気学会調査専門委員会で過去に収集されたデータを  
NIFS-DBサーバで公開  
(故)林真先生の未発表データの整理と公開(NIFS-DBサーバ/NIFS-DATA) 中村義春 慶応大

電気学会 調査専門委員会

「荷電粒子、励起種、解離種ならびに光子と原子分子ダイナミクス」  
平成18年～平成20年（代表:伊藤晴雄 千葉工大）

# 電気学会調査専門委員会で収集されたデータをNIFS-DBサーバで公開 (<http://dpsalvia.nifs.ac.jp/DB/IEEJ/>)

**Recommended data for atoms and molecules**

The recommended data set is available in the *The Institute of Electrical Engineers of Japan Report #853, Sep. 2001*. The data are reproduced measurements of Boltzmann code.

**How to get data set**  
Click name of atom/molecule

*Atom*  
[He](#), [Ne](#), [Ar](#), [Kr](#), [Xe](#), [Rb](#)

*Diatomic molecule*  
CO, N<sub>2</sub>, NO, [O<sub>2</sub>](#)

*Triatomic molecule*  
[CO<sub>2</sub>](#)

*Polyatomic molecules*  
CF<sub>4</sub>, [CH<sub>4</sub>](#), [GeH<sub>4</sub>](#), [SiH<sub>4</sub>](#), C

**Structure of data file**

For example, data file of Ar

```

890621 39.948 8      dates, atomic
elastic momentum transfer
40 0 2.746470e-005  number of data
0.000 6.300        electron energy
0.010 4.500
0.014 3.880
0.017 3.560
.
    
```

900310	131.30000	16
elastic momentum transfer		
80	.000000E+00	.829150E-05
.00000	131.00000	
.00100	123.00000	
.00250	113.00000	
.00500	99.00000	
.01000	84.30000	
.02000	67.10000	
.03000	55.70000	
.04000	47.20000	
.05000	40.80000	
.06000	35.33000	
.08000	27.84000	
.10000	22.60000	
.12000	18.10000	
.14000	14.66000	
.16000	11.97000	
.18000	9.86000	
.20000	8.18000	
.22000	6.82000	
.24000	5.73000	
.26000	4.83000	
.28000	4.10300	
.30000	3.50400	
.32000	3.01000	
.34000	2.60000	
.36000	2.26000	
.38000	1.98000	
.40000	1.74000	
.42000	1.55000	
.44000	1.38000	
.46000	1.25000	
.48000	1.14000	
.50000	1.04200	
.54000	0.90000	
.58000	0.75000	

[1] Y. Nakamura and M. Kurachi, *J. Phys.D*, **21** (1988) 718 - 723  
 [2] M. Hayashi and S. Ushiroda, *J. Chem. Phys.*, **78** (1983) 2621 - 2625  
 [3] A. Chutjian and D. C. Cartwright, *Phys. Rev. A*, **23** (1981) 2178 - 2193  
 [4] D. Rapp and P. Englander-Golden, *J. Chem. Phys.*, **43** (1965) 1464 - 1479

**Fig.1 Recommended cross sections for Ar**

**Acknowledgment**

This database is opened under auspice of the technical society "dynamics of atoms and molecules interacting with charged particles, excited species, dissociated species, and photons" of The Institute of Electrical Engineers of Japan.

Copyright (c) 2008 National Institute for Fusion Science

## (故)林真先生の文献データベース公開について

67種の原子分子について1900年から1999年(20世紀)の間に報告された文献を網羅.

そのうち、17の原子分子についてはすでにNIFS-DATA-72(Ar), -74(CO<sub>2</sub>), -76(SF<sub>6</sub>), -77(N<sub>2</sub>), -79(Xe), -80(F<sub>2</sub>, Cl<sub>2</sub>, Br<sub>2</sub>, I<sub>2</sub>), -82(H<sub>2</sub>), -83(HF, HCl, HBr, HI), -87(NH<sub>3</sub>, PH<sub>3</sub>), -90(CH<sub>4</sub>)として発行.

未発表データはNIFS-DBサーバ上で公開(準備中).

# 原子分子データベース協会

- NIFS一般共同研究の枠組みで準備会
  - 代表: 季村峯生先生(九大)が今年2月逝去、佐々木明氏(JAEA関西)が新代表に就任
- 原子分子専門家とデータユーザー、学会と産業界など、様々な観点から協会のあり方を検討中.

**IAEA Advisory Group Meeting on  
"Technical Aspects of Atomic and Molecular Data  
Processing and Exchange (19th Meeting of the  
Atomic and Molecular Data Centres and ALADDIN  
Network)"**

**3-5 October 2007, IAEA Headquarters, Vienna, Austria  
Scientific Secretary: D. Humbert**

**IAEA 1<sup>st</sup> Coordination Research Meeting on  
"Data for surface composition dynamics relevant to  
erosion processes"**

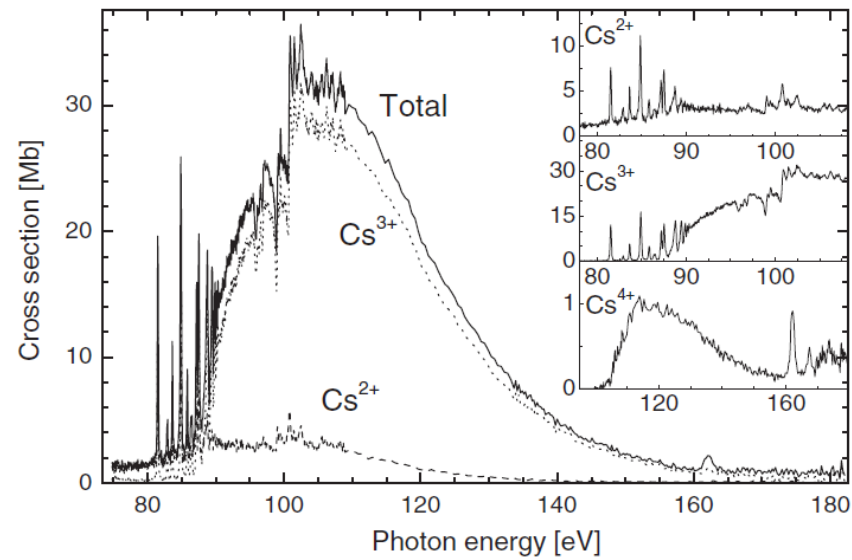
**17-19 October 2007, IAEA Headquarters, Vienna,  
Austria  
Scientific Secretary: R.E.H. Clark**

# 予備

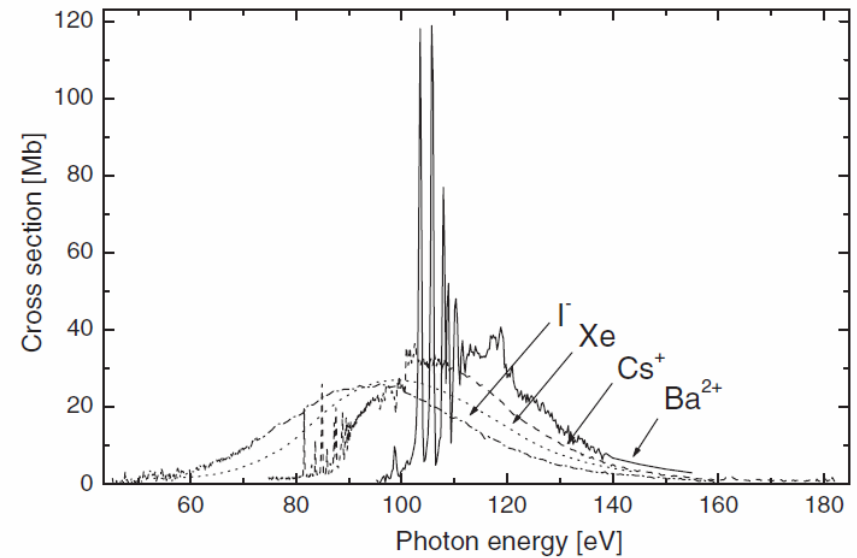


# Photo-ionization cross section of Ions

Cs<sup>+</sup>



Iso-electronic sequence



H. Kjeldsen, P. Andersen, F. Folkmann, J. E. Hansen, M. Kitajima, and T. Andersen, J. Phys. B. **35**, 2845 (2002)

## FP3-3 Standardization of atomic and molecular data for fusion research

Yu. Ralchenko (Univ. of Maryland College Park, USA),

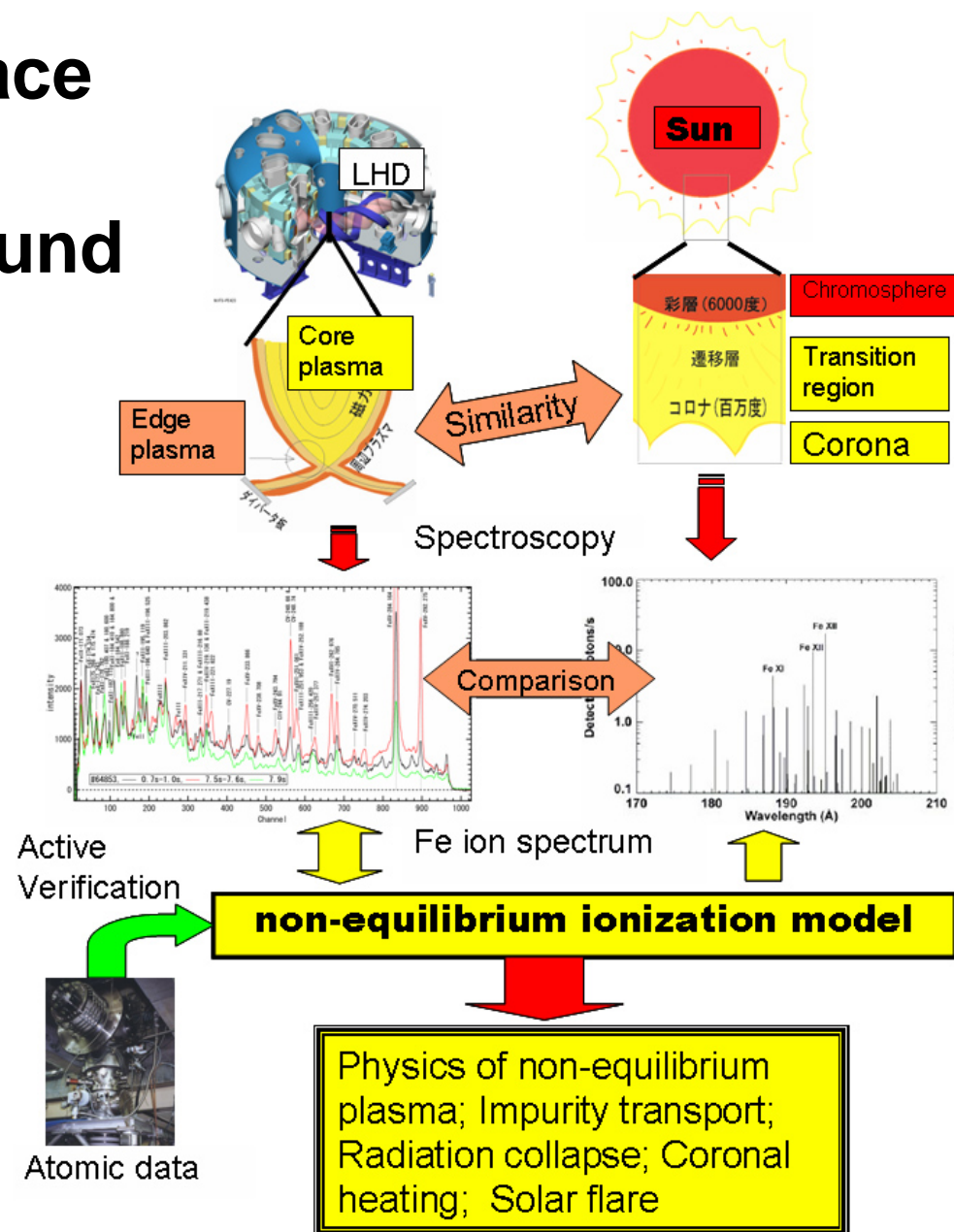
I. Murakami, D. Kato (NIFS)

2006 Nov. 29- Dec. 9

- Related to recent movement on new atomic and molecular database network with **Atomic and Molecular Data Markup Language (AMDML)**.
- Current Atomic Data Search Engine (GENIE) by IAEA is just merging outputs from each database and unified format is required.
- To develop an **XML schema allowing for a complete description of atomic, molecular, and particle-surface (solid) interactions and properties, and other tools (Web services)** for data exchange.
- Development approved by the IAEA Data Center Network
- Currently active: **NIST, IAEA, ORNL, Paris Observatory, NFRC(Korea) will join**
- Presently finalizing the XML Schema
- Other related projects are under discussion
- **New search engine system** will communicate with each database through a gate with AMDML of unified XML schema and each database system is not needed to change its database system. "A new gate" system is just required.
- NIFS will be able to contribute to checking the XML schema and joining the new network.

# Investigate the Space through the Sun on the Ground

1. Construct **Collisional Radiative Model** for Fe L and M shell ions
2. Produce and evaluate atomic data for Fe ions
3. Measure spectra from **LHD**, analyze them by **non-equilibrium ionization model** and verify our model.
4. Apply our model to **solar spectra** measured by the “Hinode” satellite to understand coronal heating mechanism.



**IAEA Advisory Group Meeting on  
"Technical Aspects of Atomic and Molecular Data Processing and  
Exchange (19th Meeting of the Atomic and Molecular Data Centres and  
ALADDIN Network)"**

**3-5 October 2007, IAEA Headquarters, Vienna, Austria**

**Scientific Secretary: D. Humbert**

Wednesday, 3 October

**Meeting Room: A2774**

09:30 - 09:45 Opening (R.E.H. Clark, Head, A+M Data Unit, A. Nichols, Section Head, Division of Physical and Chemical Sciences, NAPC)

Adoption of Agenda

**Session 1.** Current Activities of the A+M Data Centres

Chairman: J Yan

09:45 - 10:30 W. Eckstein (MPIP)

10:30 - 11:00 **Coffee break**

11:00 - 11:45 Yu.V. Martynenko (Kurchatov Institute)

11:45 - 12:30 G. Mazzitelli (ENEA)

12:30 - 14:00 **Lunch**

**Session 2.** Current Activities of the A+M Data Centres (Continued.)

Chairman: Y. Rhee

14:00 - 14:45 D. Kato (NIFS)

14:45 - 15:30 D. Humbert (IAEA)

15:30 - 16:00 **Coffee break**

16:00 - 16:45 A. Whiteford (ADAS)

Thursday, 4 October

**Session 3.**

Chairman: W. Eckstein

9:00 - 9:45 D.R. Schultz (ORNL)

9:45 - 10:30 Y. Rhee (KAERI)

10:30 - 11:00 **Coffee break**

11:00 - 11:45 K. Katsonis (GAPHYOR)

11:45 - 12:30 W.L. Wiese (NIST)

12:30 - 14:00 **Lunch**

**Session 4.** Current Activities of the A+M Data Centres (Continued.)

Chairman: K. Katsonis

14:00 - 14:45 T. Nakano (JAEA)

14:45 - 15:30 J. Yan (CRAAMD)

15:30 - 16:00 **Coffee break**

16:00 – 16:45 D. Kato “ITER AM/PSI Data Needs”

16:45 - 17:15 Yu. Ralchenko (NIST) “XML Format for A+M Data”

Friday, 5 October

**Session 5.**     Data Issues

Chairman:     W. Wiese

9:00 - 10:45     Priorities in A+M data compilation (all participants)  
Data evaluation (all participants)  
Data for the Int. Bulletin on Atomic and Molecular Data for Fusion

10:45 - 11:15     **Coffee break**

**Session 6.**

Coordination:   R.E.H. Clark and D. Humbert

11:15 - 12:45     Review of Data Center Network Membership criteria  
Membership of Brazil and ADAS  
Plan of DCN activities for the near future  
ICAMDATA

12:45 - 14:00     **Lunch**

**Session .7**     Demonstrations

14:00 – 15:30     Data Centre WWW and software demonstrations

15:30 - 16:00     **Coffee break**

**Session 8:**     Meeting Conclusions and Recommendations

Chairman:     D. Humbert

16:00 - 17:00     Formulation of meeting conclusions and recommendations  
Date of next meeting

**17:00 -**         **Adjourn of the Meeting**