重粒子衝突物理と近代技術の基礎

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If, in some cataclysm, all of scientific knowledge were to be destroyed, and only one sentence passed on to the next generations of creatures, what statement would contain the most information in the fewer words? I believe it is the ***atomic hypothesis*** (or the ***atomic fact***, or whatever you wish to call it) that ***all things are made of atoms*** **--- little particles that move around in perpetual motion, attracting each other when they are a little distance apart, but repelling upon being squeezed into one another.** In that one sentence, you will see, there is an enormous amount of information about the world, if just a little imagination and thinking are applied.

Richard P. Feynman

Outlines:

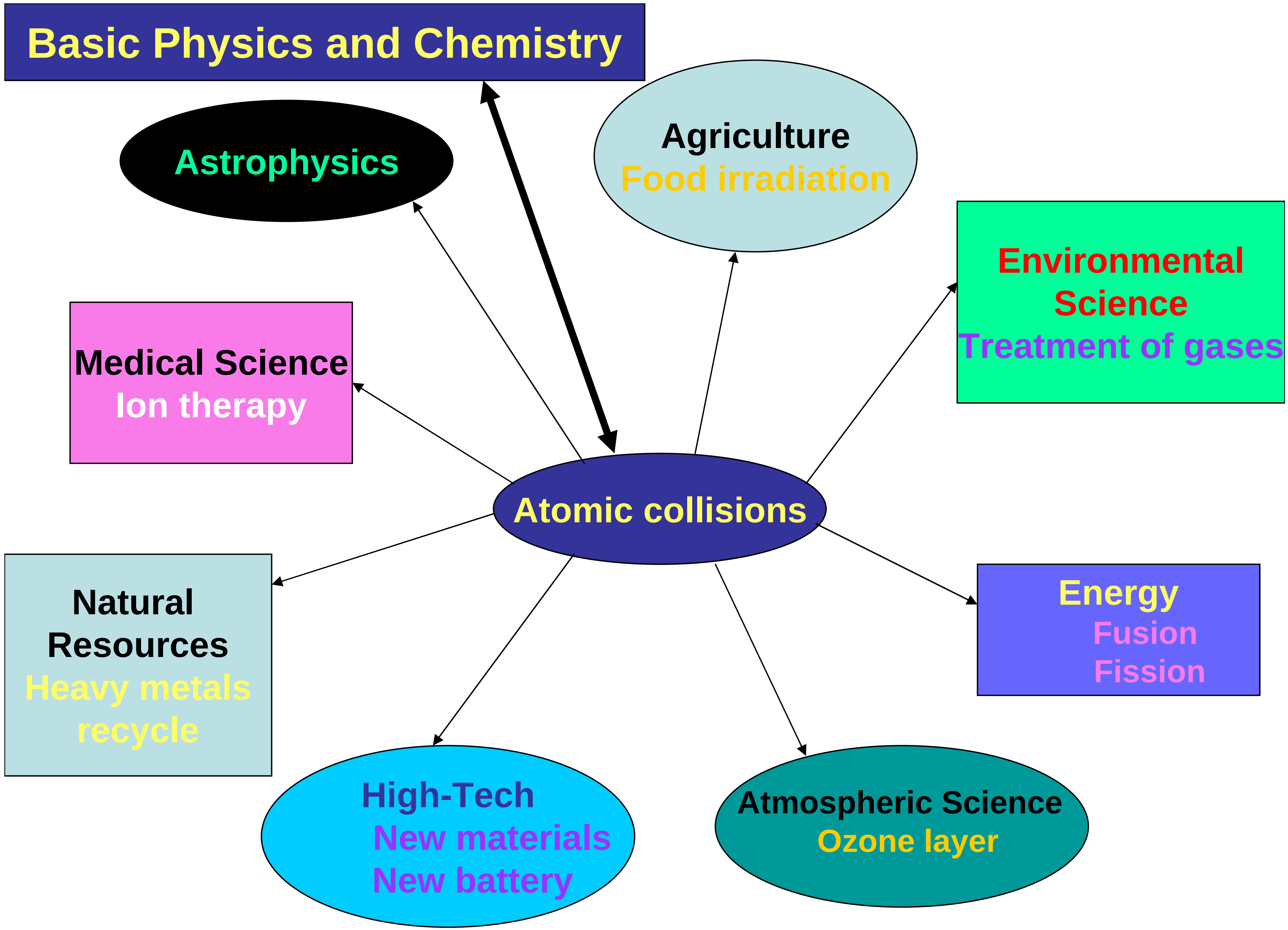
- Examples of applications
  ——What are Atomic Collisions?
- History of Atomic Collisions
- What kinds of processes in Atomic Collisions are possible?
- Theoretical frame
- What is the status of our understanding of Atomic Collisions?
- Summary and Perspectives

多様性：

半導体製造、薄膜生成、ハイテク、
核融合、レーザー、新エネルギー、
医療、環境ー大気科学、天体物理、
農業

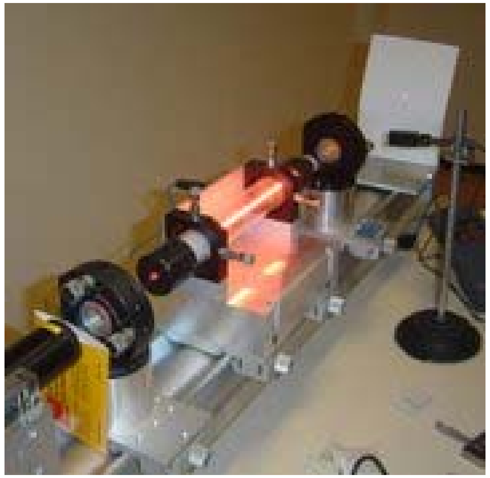
普遍性：

光・電子・イオンー物質との相互作用


Basic Physics and Chemistry
Astrophysics
Agriculture
Food irradiation
Environmental Science
Treatment of gases
Medical Science
Ion therapy
Atomic collisions
Natural Resources
Heavy metals recycle
Energy
Fusion
Fission
High-Tech
New materials
New battery
Atmospheric Science
Ozone layer

Applications:

- レーザー
- イオンビーム蒸着
- 核融合
- 医療ーガン治療
- 天体物理
- 材料分析ーPIXE



レーザー

原子衝突によるエネルギー移動
(Energy transfer)

- He* + Ne → He + Ne*

  └ Ne + hυ

- Excimer(励起二量体）

  A* + M → AM*

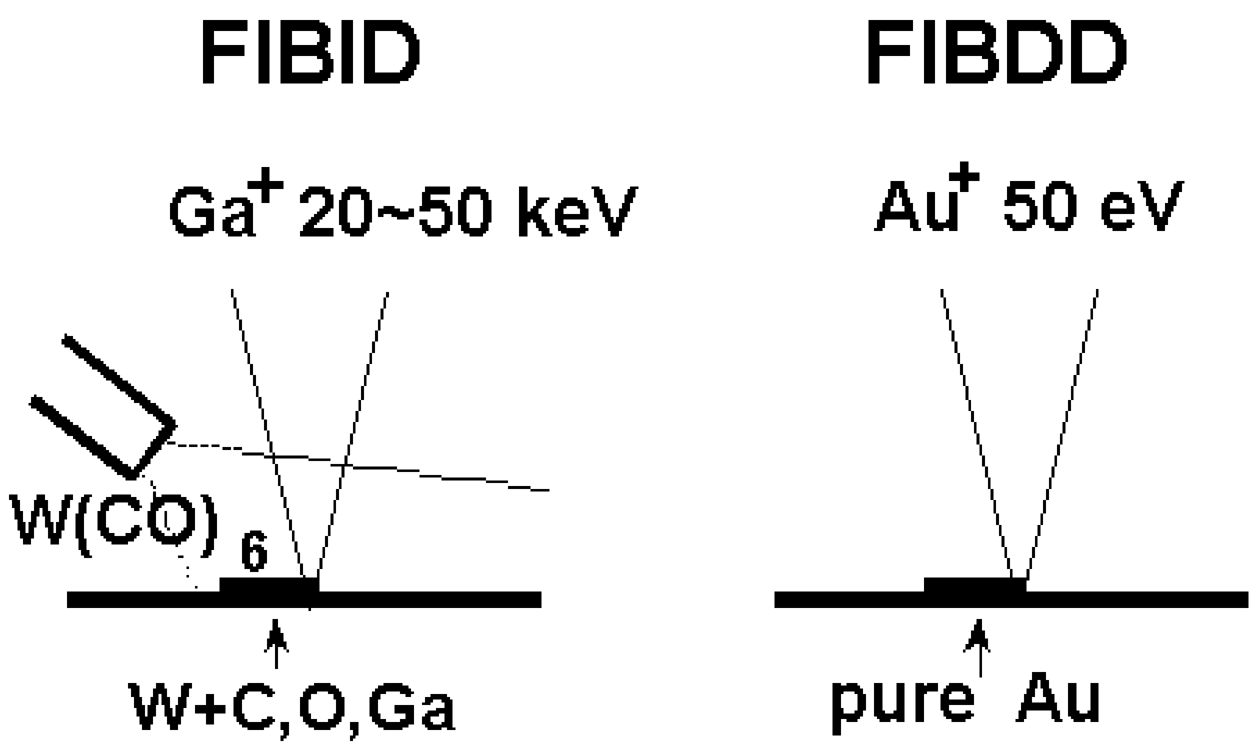
  └ A + M + hυ

  A(基底状態）~~+~~ M → AM

- CO2 Laser

  CO2(v’）→CO2(v) 振動脱励起

集束イオンビーム直接蒸着法（Focused Ion Beam Direct Deposition：FIBDD）



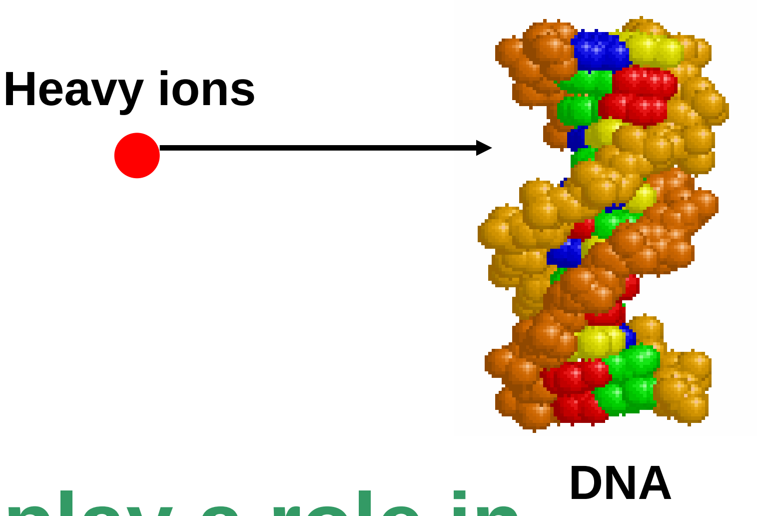
Heavy-ion Cancer Therapy:
Physics and Chemistry in the Bragg Peak

- **Heavy ions:**

  $C^{4+}(1s^2)$, C^{6+},

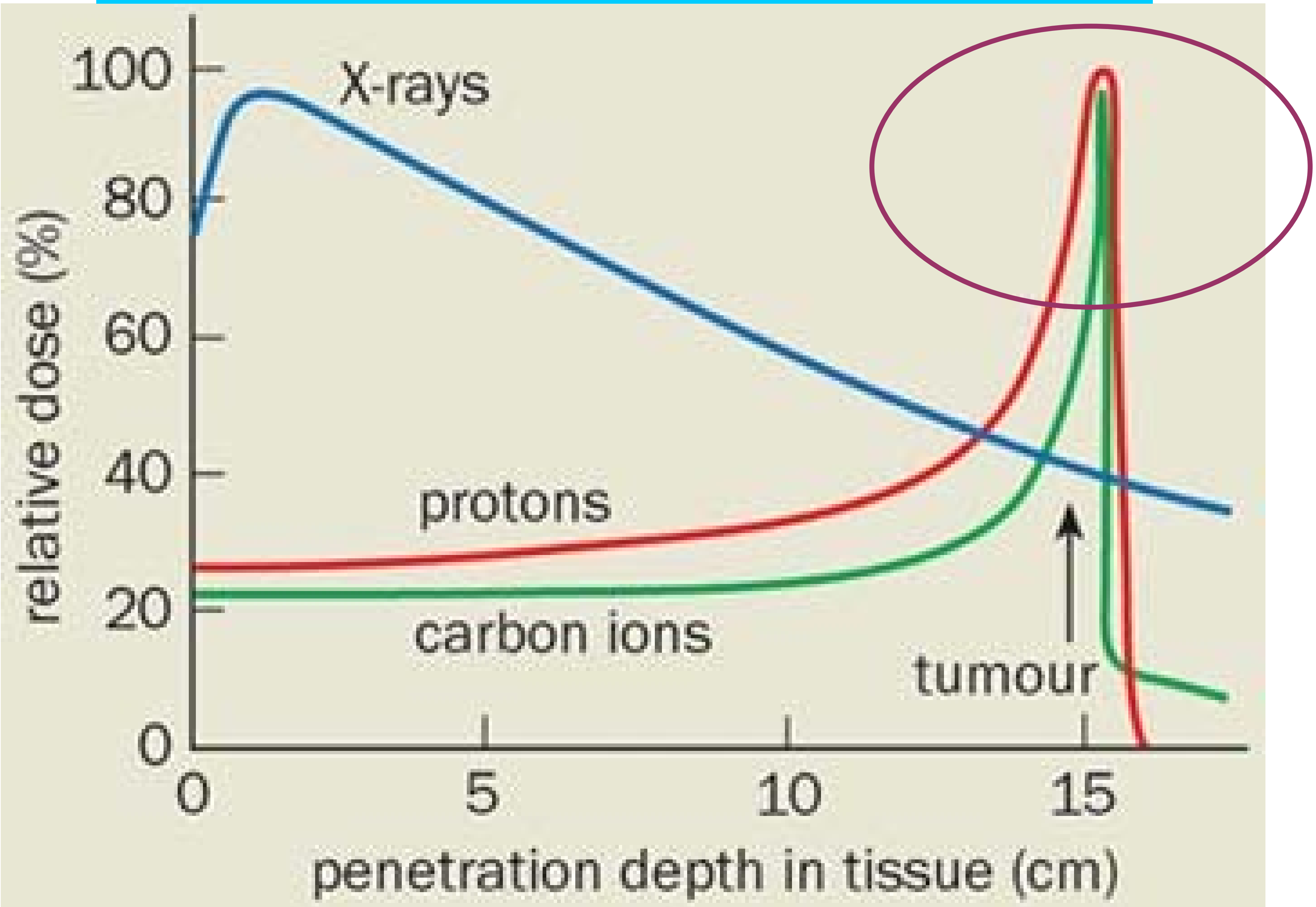
  $O^{6+}(1s^2)$, O^{8+}, Ne^{10+},

  … (heavier than proton)



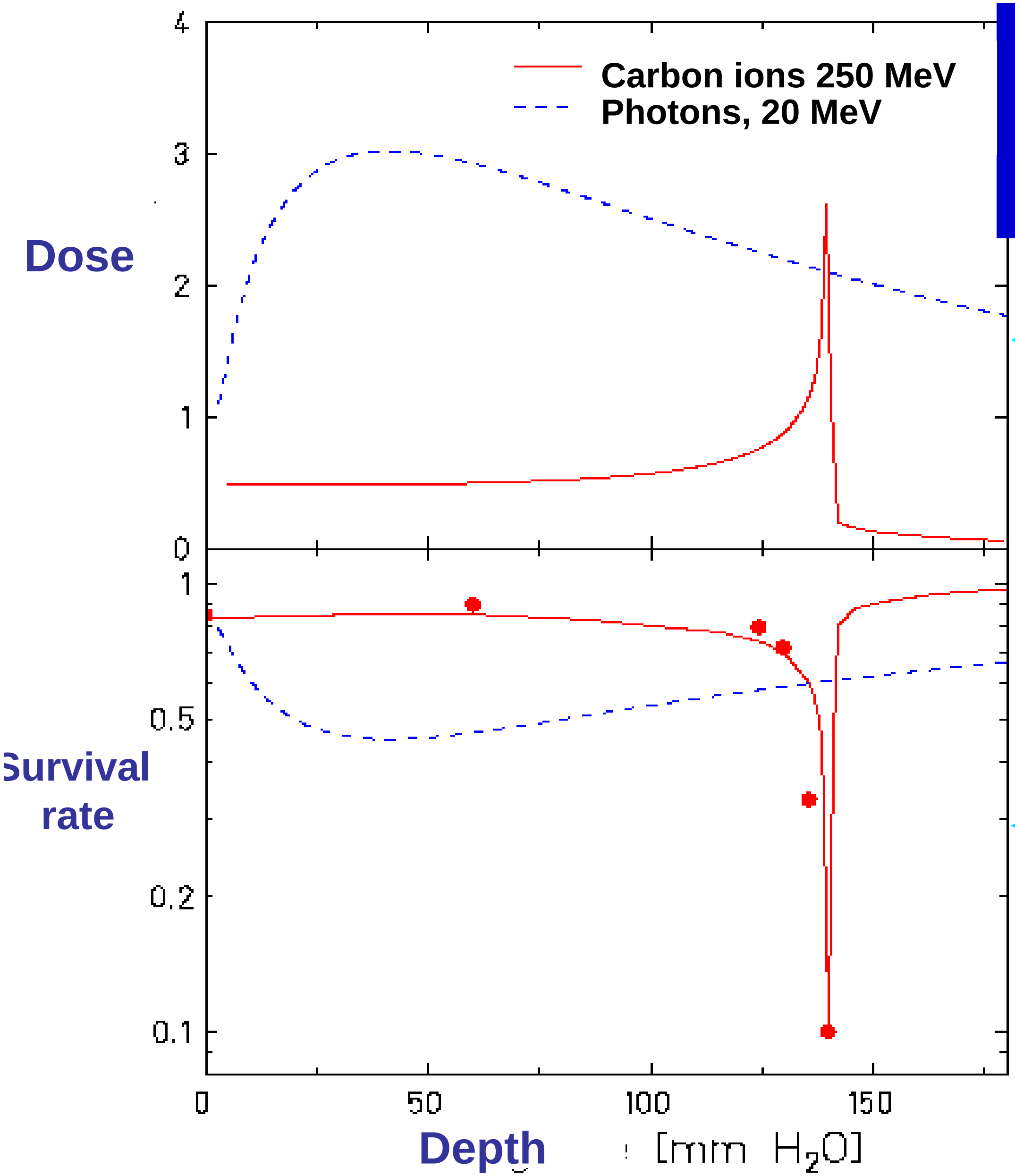
- How do Atomic Collisions play a role in dynamics?
- How do they differ from electrons and photons?

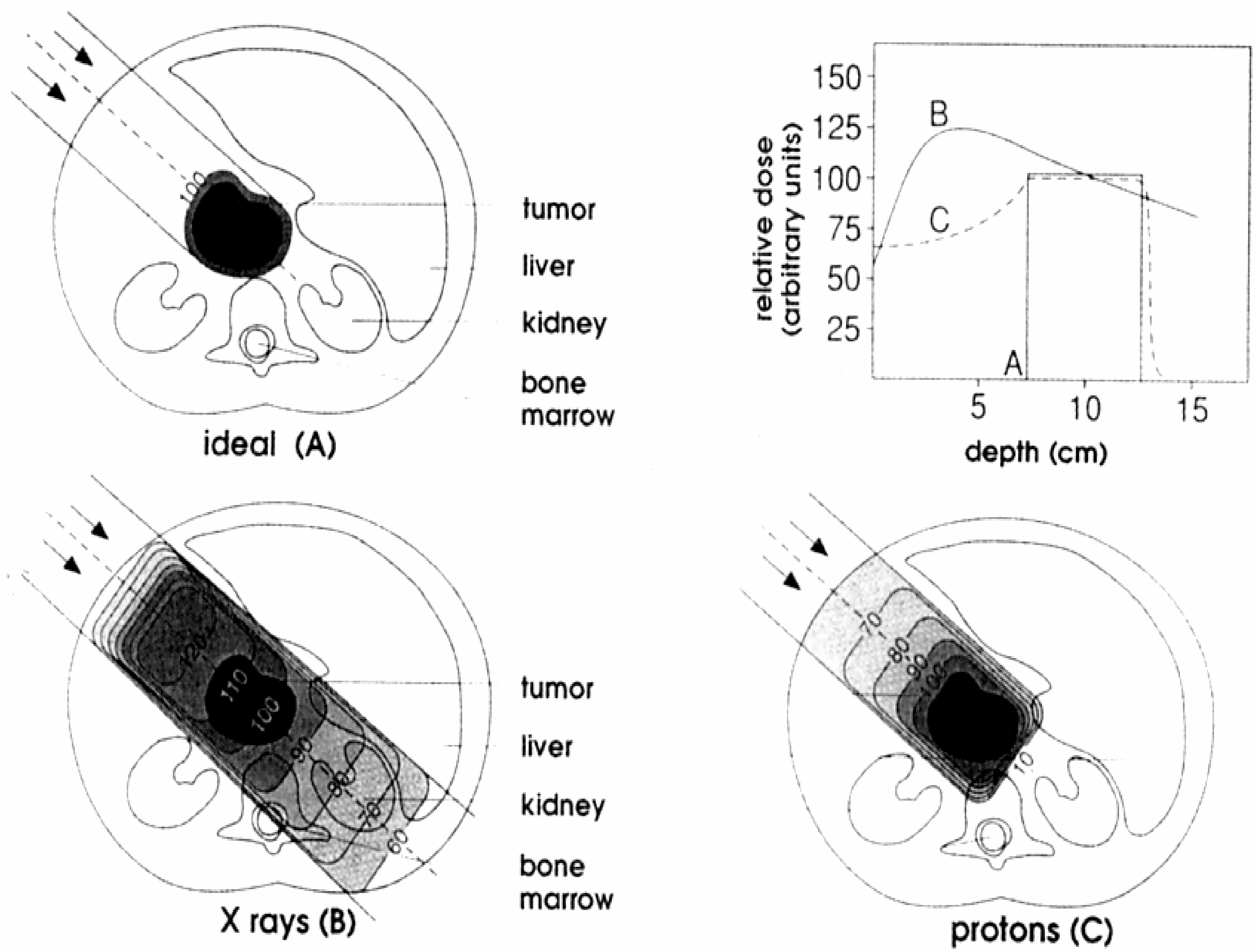
Bragg peak



100
80
60
40
20
0
relative dose (%)
X-rays
protons
carbon ions
tumour
0
5
10
15
penetration depth in tissue (cm)

Relationship between the Bragg peak and Survival rate of cells





tumor
liver
kidney
bone marrow
ideal (A)
relative dose (arbitrary units)
depth (cm)
150
125
100
75
50
25
5
10
15
A
B
C
110
100
90
80
70
60
X rays (B)
protons (C)

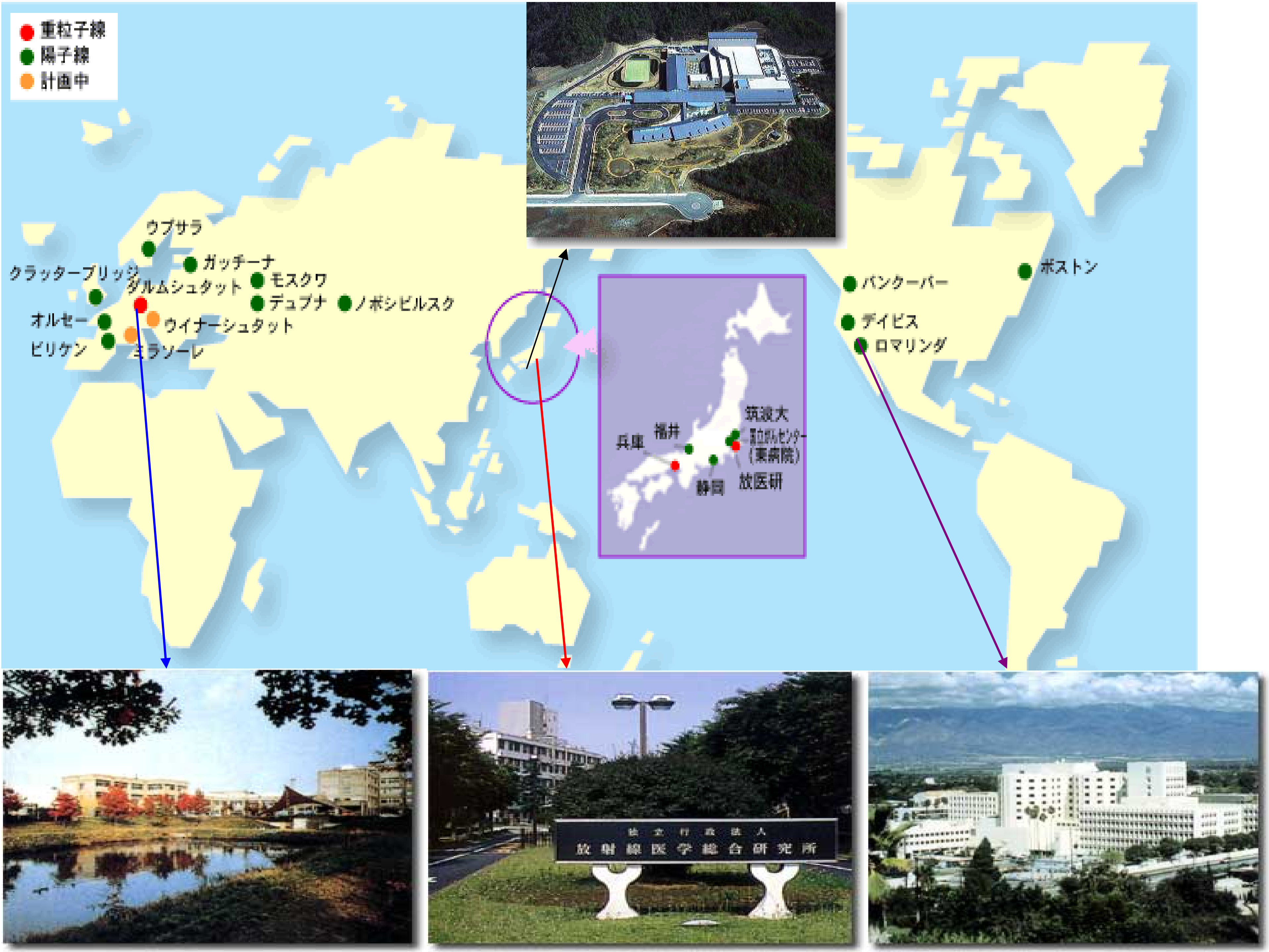
Local control rates of tumors by irradiation of C-ion、X-ray and neutron：

	C4+ (%)	X-ray+Chemo (%)	Neutron (%)
Salivary gland	80	28	60-70
Nasopharynx	63	21	50-80
Sarcoma	56	28	54
Prostate	100	60-70	77
Lung	39	22-40	----
Brain	44	18	----

Problems of Heavy-ion therapy

- **Exceedingly expensive!**

Heavy-ion (HIMAC)	$400 M
Proton	$50—100M
X-ray	$10M


重粒子線
陽子線
計画中
ウプサラ
クラッターブリッジ
ダルムシュタット
ガッチーナ
モスクワ
デュブナ
ノボシビルスク
オルセー
ウイナーシュタット
ビリケン
ミラソーレ
兵庫
福井
筑波大
(東病院)
静岡
放医研
バンクーバー
ボストン
デイビス
ロマリンダ
放射線医学総合研究所

Physics and Chemistry of Heavy ion therapy

- **Heavy ions:**

  H^{+},.....,$C^{4+}(1s^2)$, C^{6+}, $O^{6+}(1s^2)$, O^{8+}, Ne^{10+},... Ar,.......

- **Energy:**

  > ~250 MeV

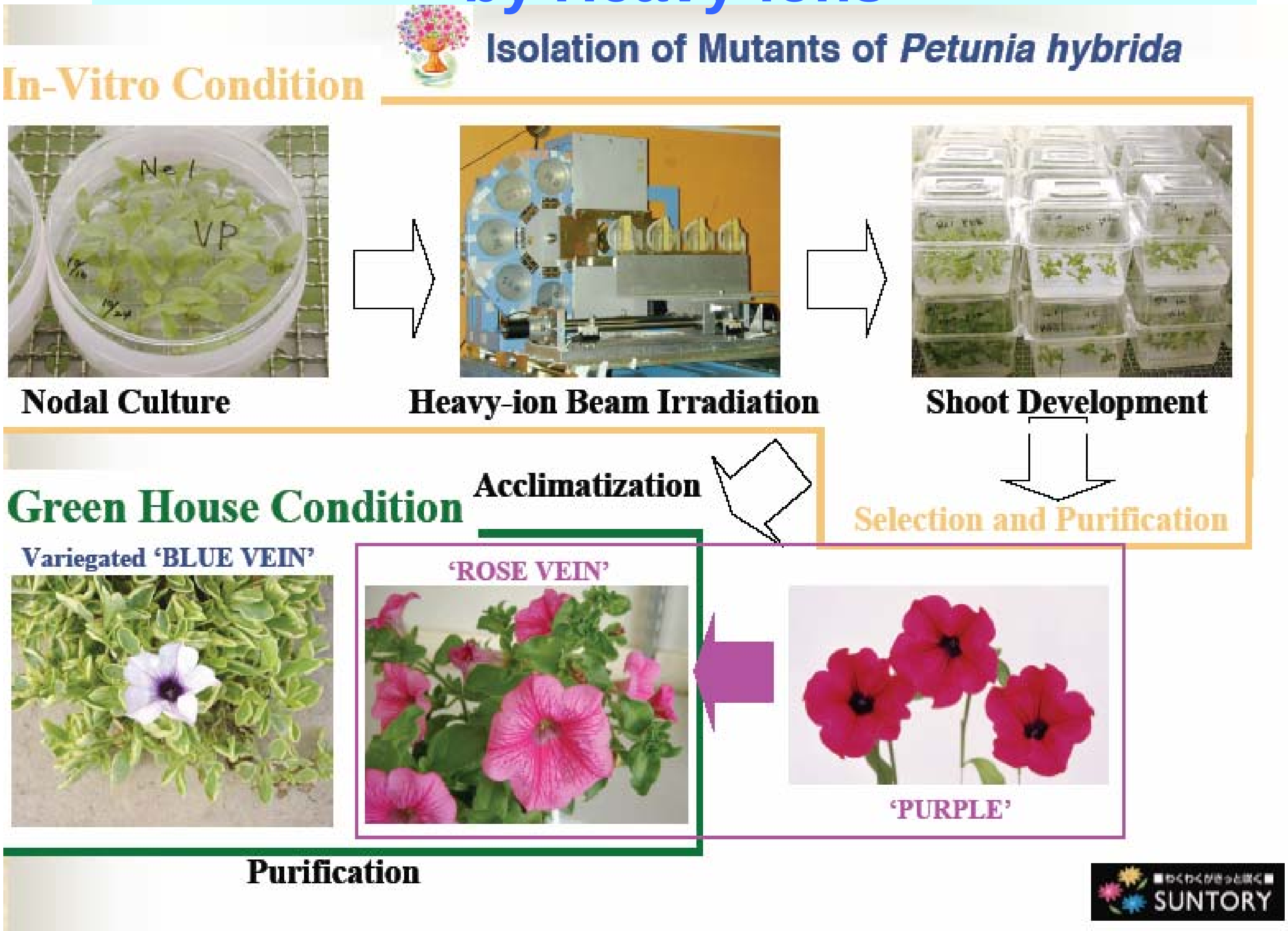
▸ **What are ion-biomolecule interactions?**

Example of Ion—Molecule Collisions:

$H^+ + H_2(n, v, J)$	$\rightarrow H^+ + H_2\,(n, v, J)$	Elastic scattering
	$\rightarrow H^+ + H_2^+\,(n', v', J') + e$	Ionization
	$\rightarrow H^*(n) + H_2^+\,(n', v', J')$	Electron capture
	$\rightarrow H^+ + H_2^*(n^*)$	Electronic excitation
	$\rightarrow H^+ + H_2(n'', v'', J'')$	Ro-vibrational excit.
	$\rightarrow H_2^{+(*)} + H$	Chemical reaction
	$\rightarrow H_3^+ + h\nu$	Association

n, v, J: Electronic, vibrational, rotational QN

Development of New Plant Species by Heavy-ions

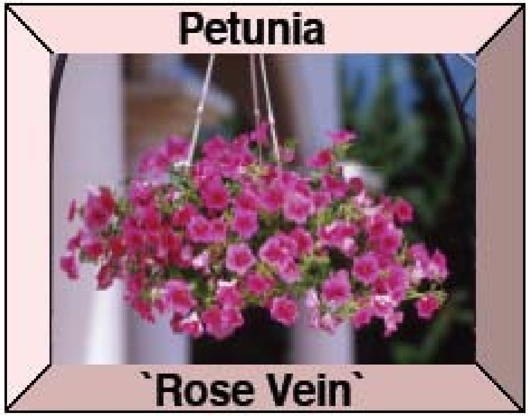


New Plants by Heavy-ions

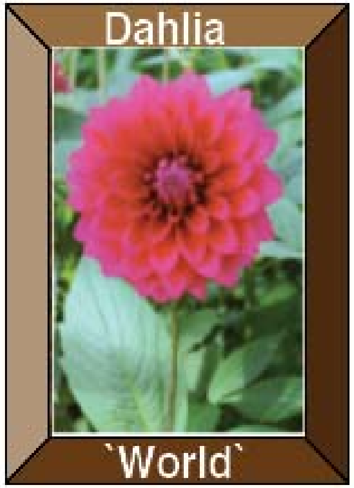
Mutation breeding using heavy-ion beam irradiation

Tomoko ABE
Plant Functions Lab., RIKEN

Petunia



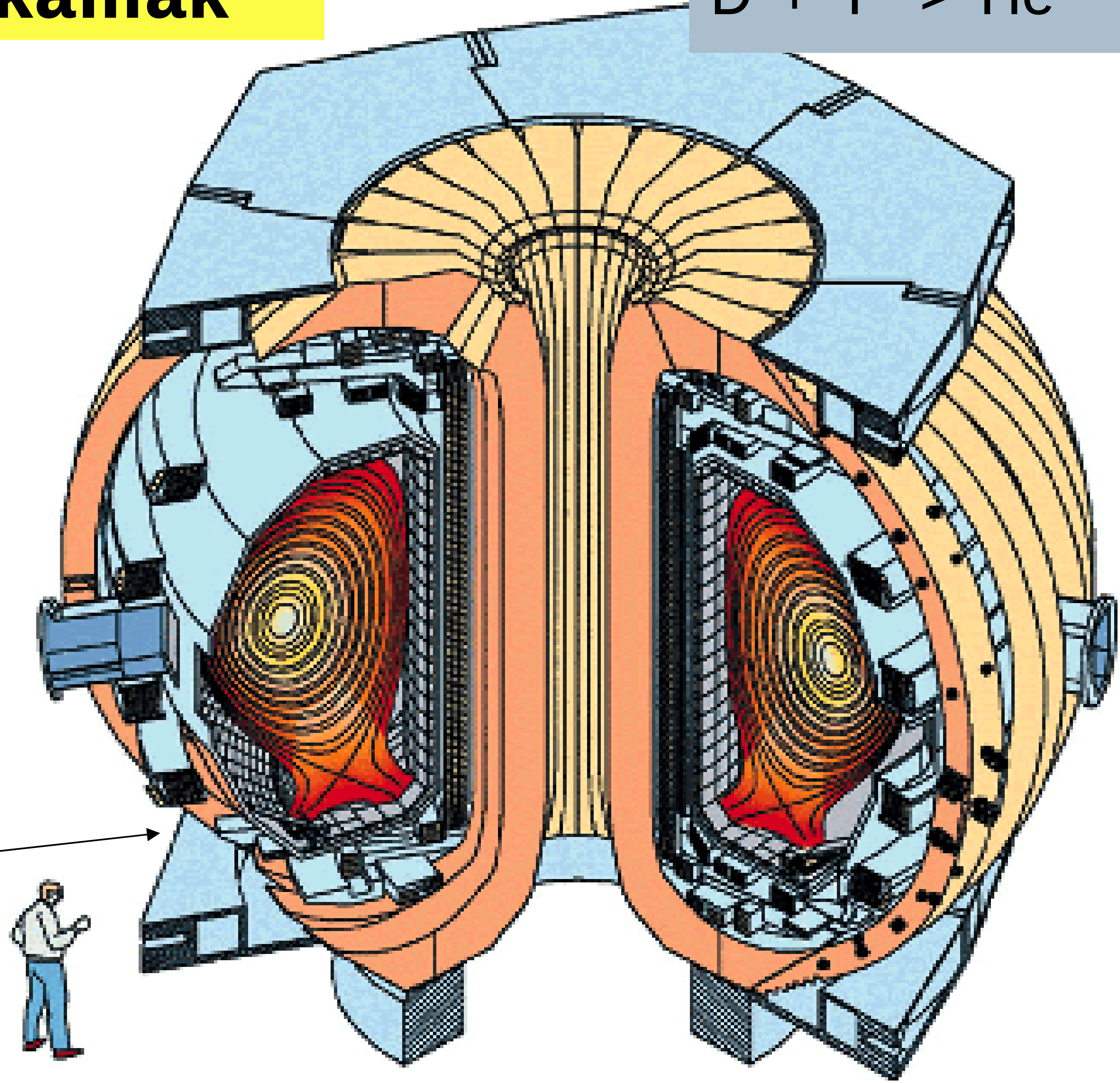
Suntory Flowers Ltd.



Hiroshima City
Agr.Forest.Promot.Cen.

Tokamak

$D + T \rightarrow He^{++} + n$



核融合の原理

- D + T → He^{2+} + n
- プラズマ温度

  中心:1億度　(数10 keV)

  エッジ:＞常温　(＞数 eV)
- 成分

  主プラズマ:電子、陽子(p)、He2+

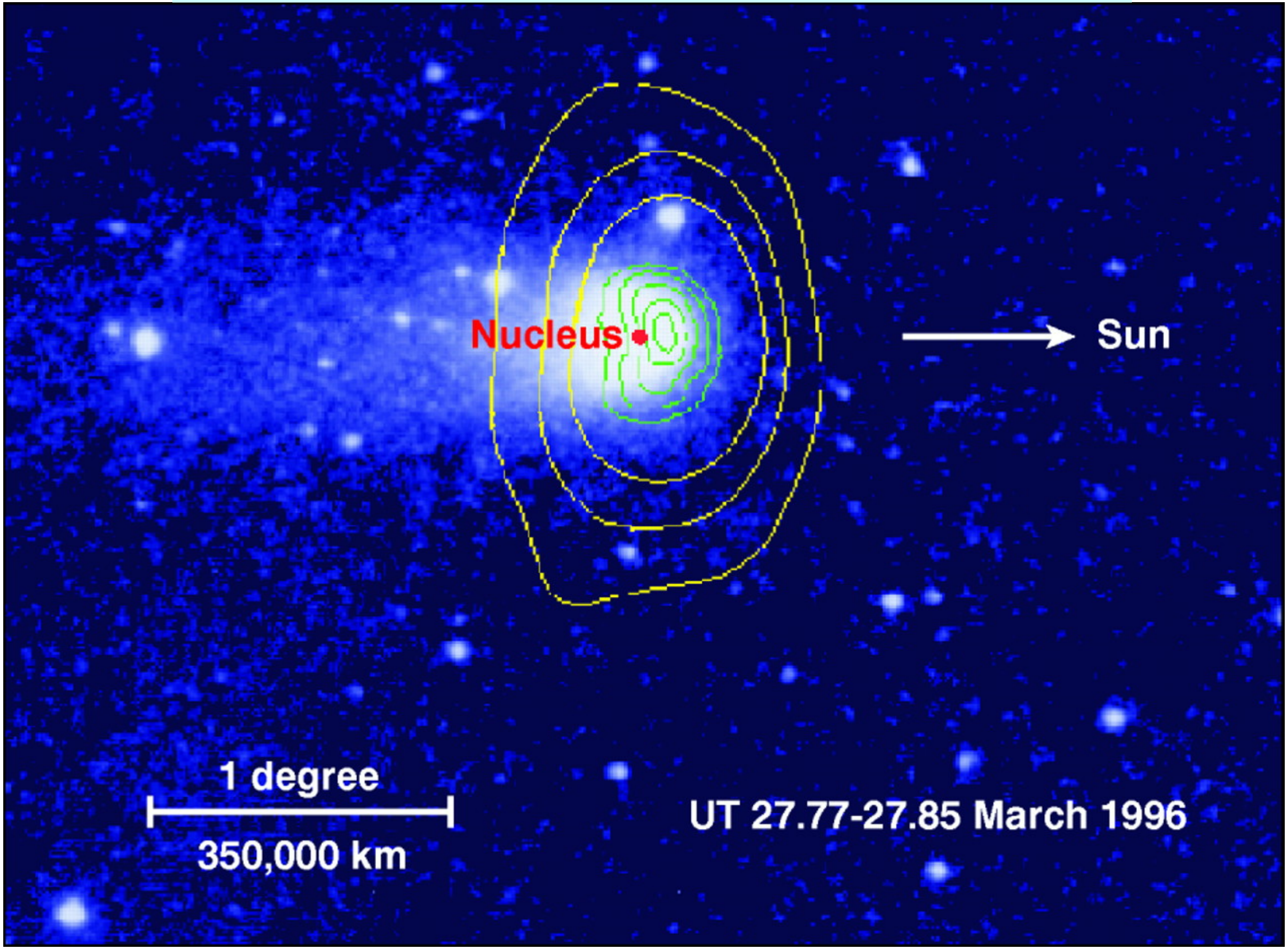
  不純物プラズマ:C^{q+}, O^{q+},……..

  不純物:炭化水素分子など

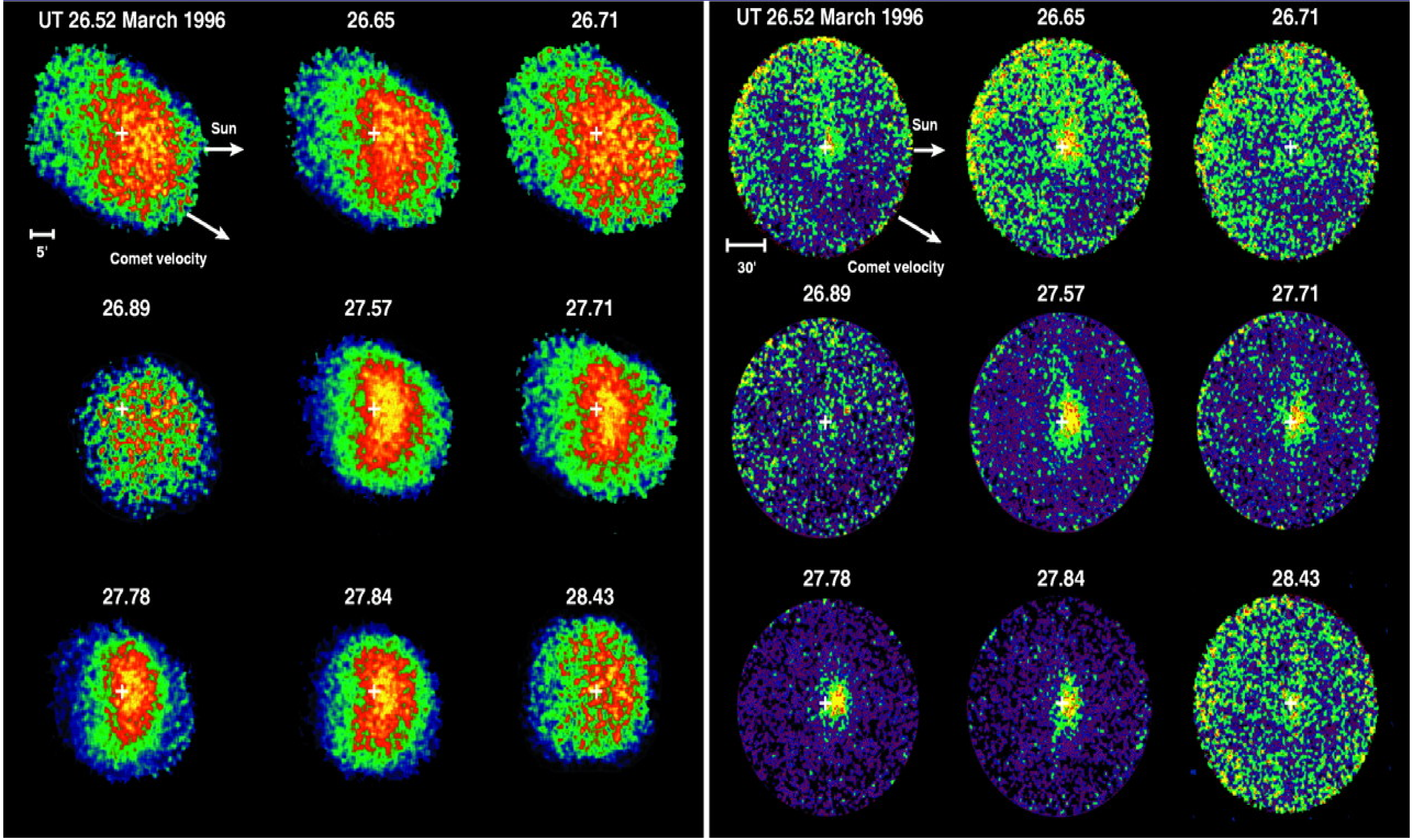
Collision processes in Fusion

- **Spectroscopy for plasma diagnostics**
  - **Ionization**
    - **Plasma production**
  - **Charge transfer**
    - **Plasma temperature and density**
    - **Impurity identification**

X-ray emission from Comets



X－ray and EUV from Comet Hyakutake



Characteristics of comets -- Dirty snowballs

- **Structure: Nucleus + Coma + H Colona + Tail (plasma + dust)**
- **Size: Nucleus(1-10km), Coma(0.1M-1M km),**

  H Colona(10M km), Tail (10M-1B km)
- **Temperature: <100-150 K**
- **Molecular compositions: H_2O, CN, CH_4, CS, CO, OH, CH, NH, H_2O^+, OH^+, CO_2^+, CO^+,……**

Origin of x-rays

OUT!!

- Electron impact
- Charge transfer by ions in solar winds

Charge transfer by heavy-ions in solar winds

- **Compositions:**

  p, He2+, Cq+, Nq+, Oq+,……. (not well known)

- **Energy:**

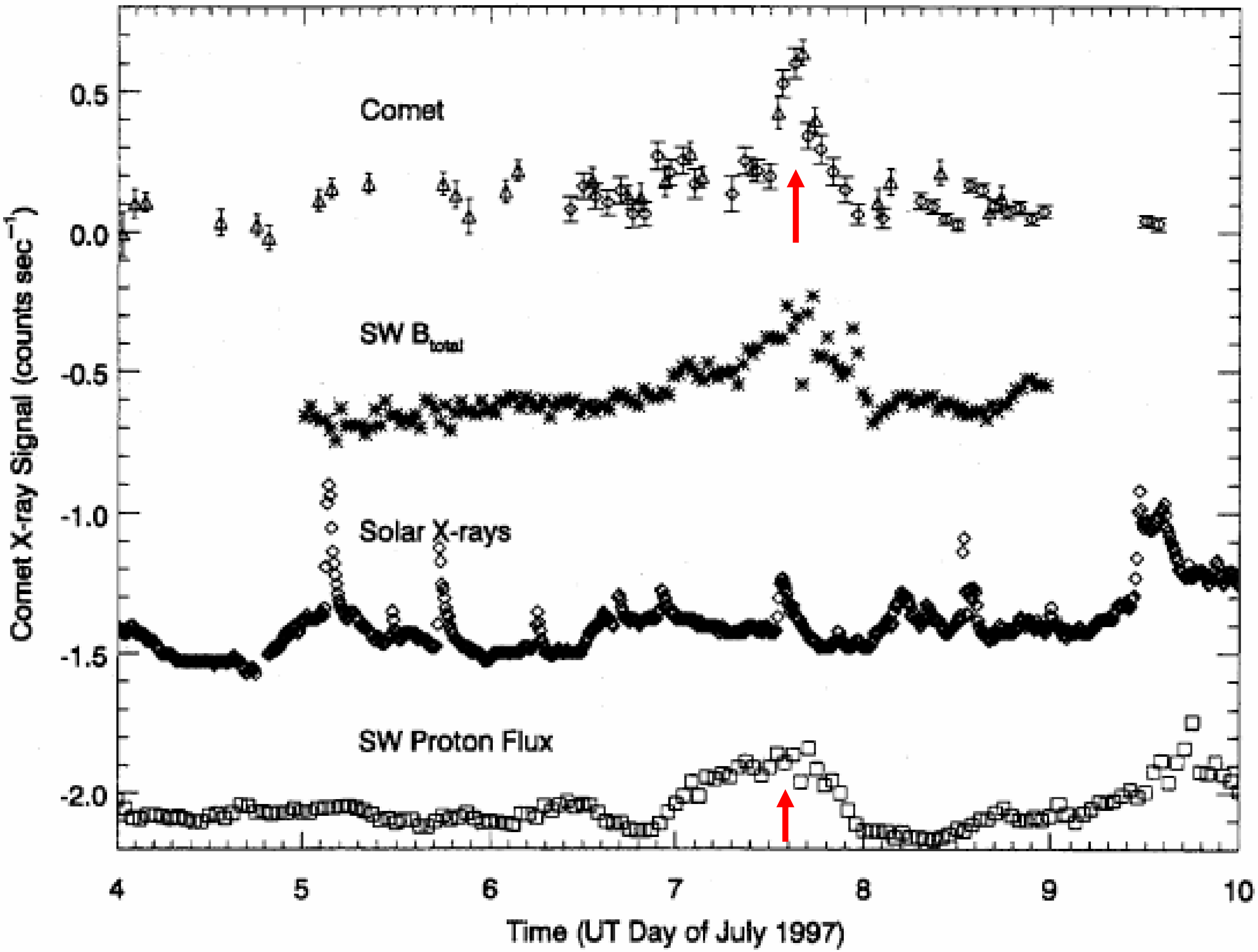
  A few 10 eV~a few keV (< 2 keV)

- **Processes:**

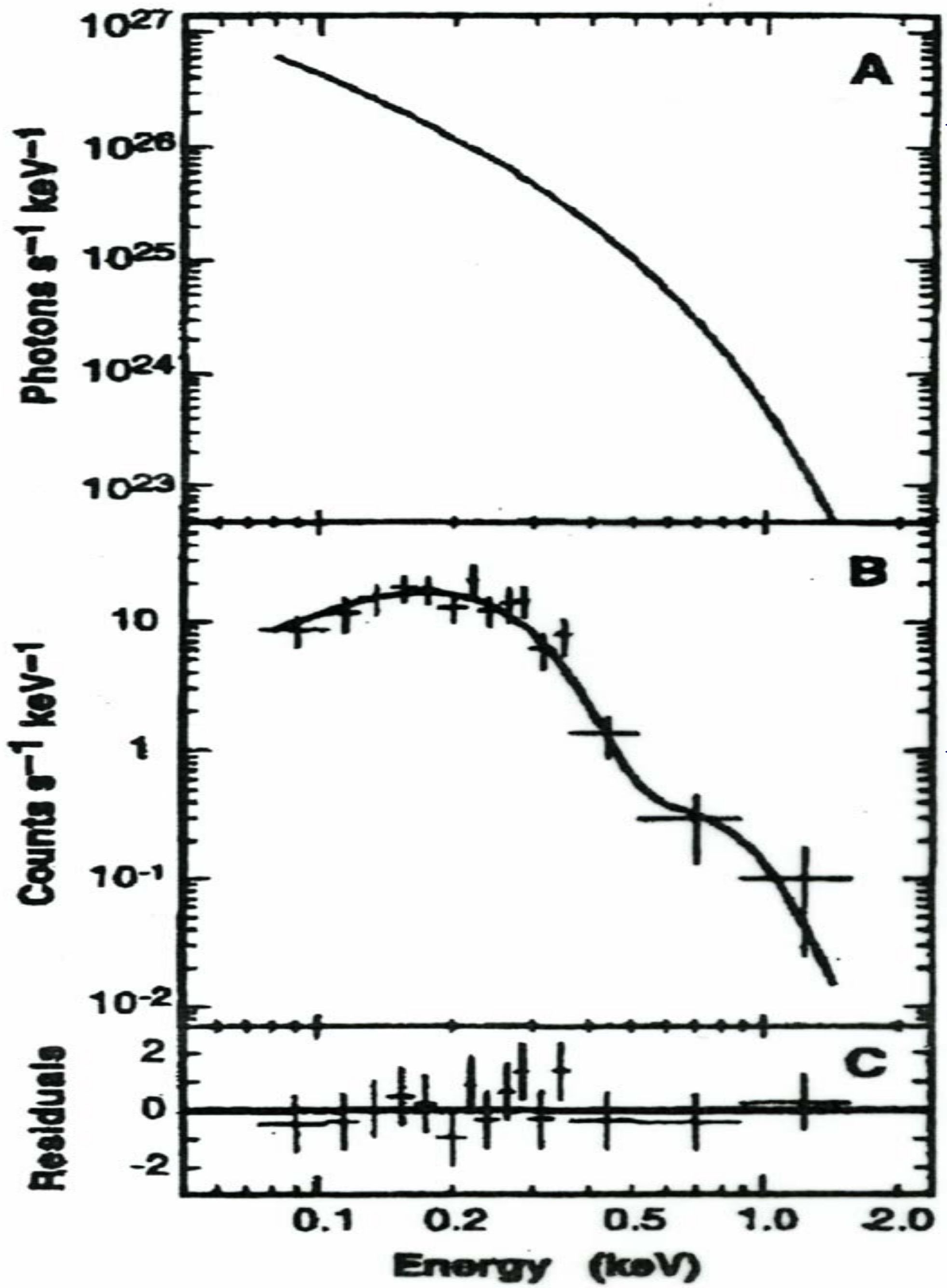
$$O^{q+} + H2O \longrightarrow O^{(q-1)+*} + H2O^{+}$$

$$\llcorner\ O^{(q-1)+} + h\upsilon$$

X-ray emission!

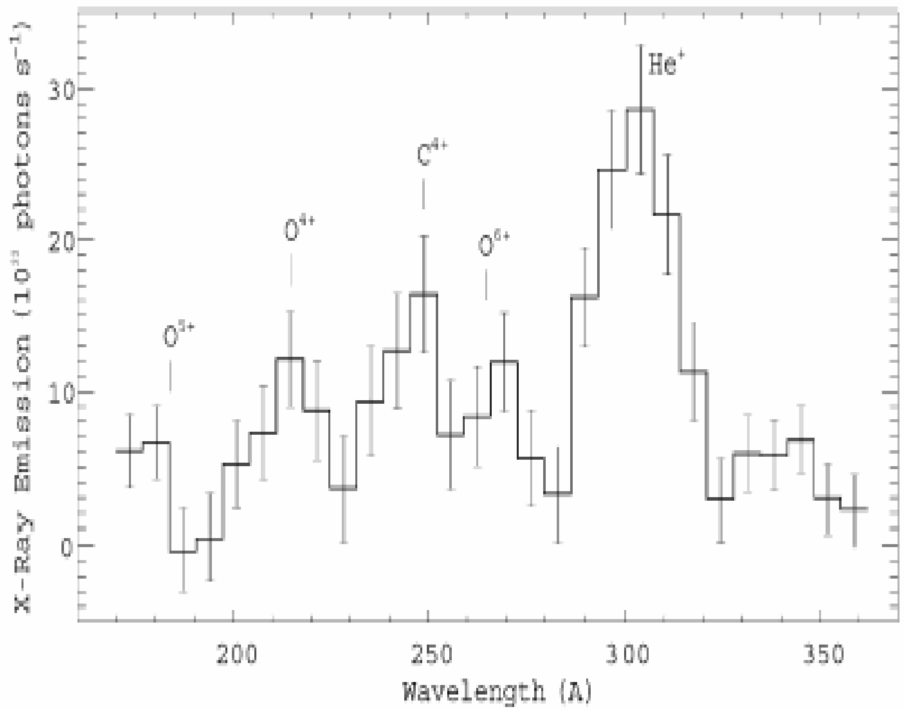


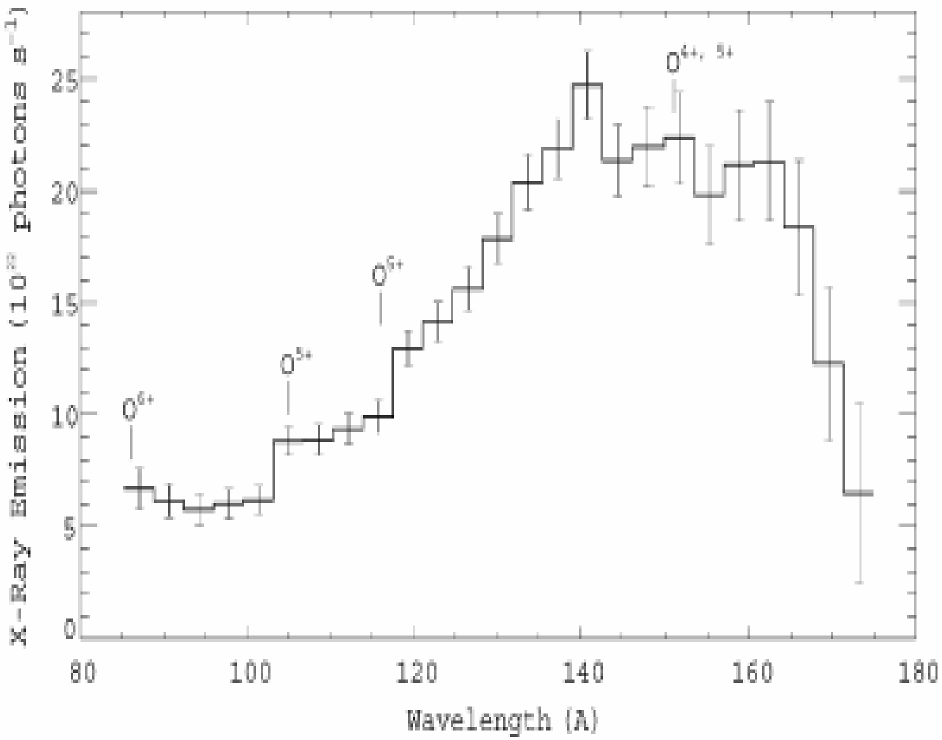
Comet
SW B$_{total}$
Solar X-rays
SW Proton Flux
0.5
0.0
-0.5
-1.0
-1.5
-2.0
Comet X-ray Signal (counts sec^{-1})
4
5
6
7
8
9
10
Time (UT Day of July 1997)

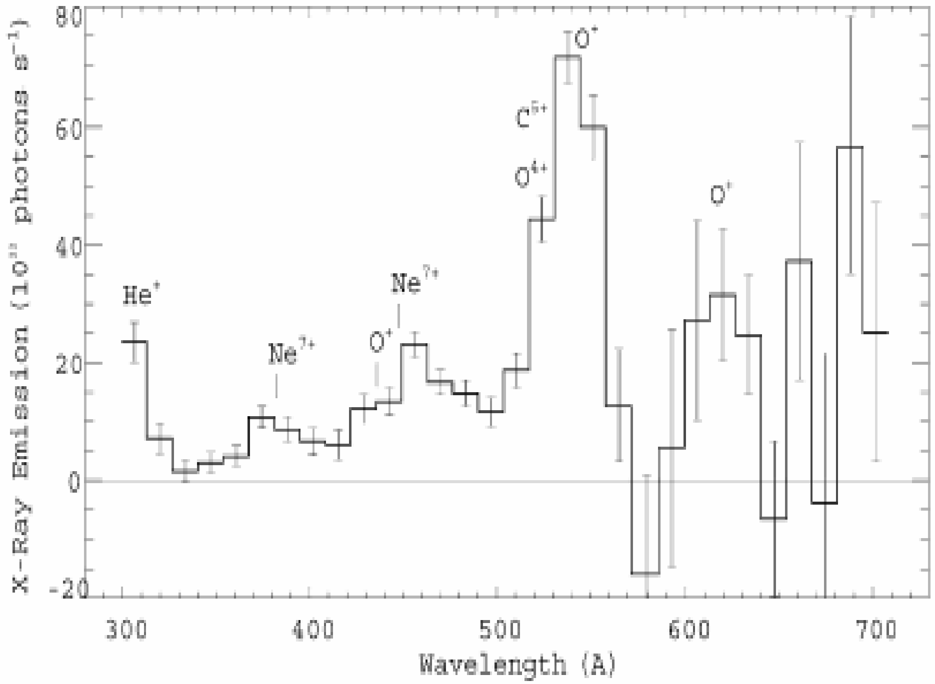


Model
based on the Bremsstrahlung

Observed spectrum

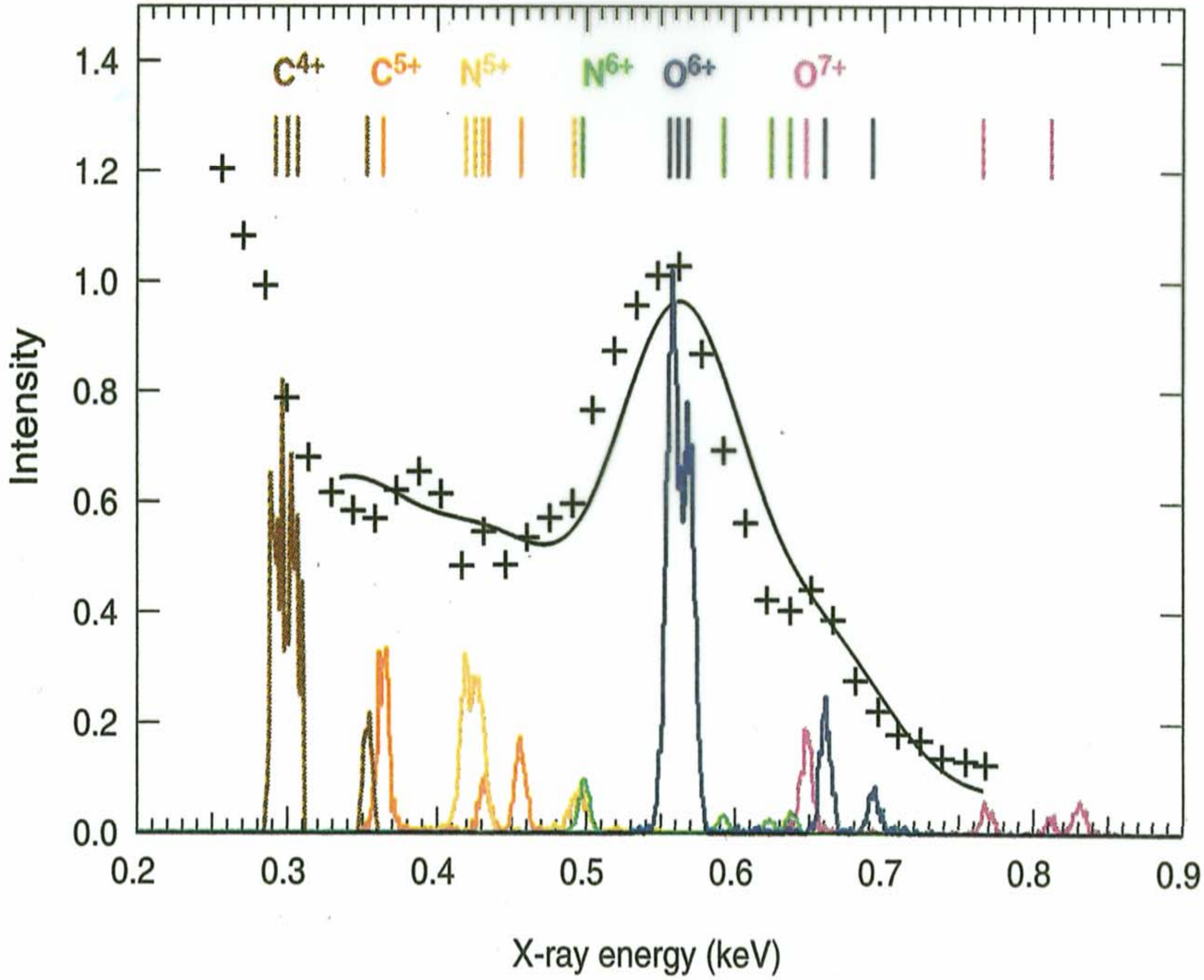






EUVE Spectrum of Hyakutake

Model calculation for SW on H2O



ハイテク技術

反応性プラズマ：電子、ラジカル、イオン

- 反応性プラズマによるエッチング
- 薄膜生成
- 材料診断——PIXE
- 環境汚染物質除去·回収·再利用

Plasma Processing

- Etching
- Fabric courting
- Thin-film
- ....

Principles of Atomic Collisions:

$e + M \rightarrow e + M^+ + e$ Ioniz.

$\rightarrow e + M^*$ Exc.

$\rightarrow M^-$ e-attachment

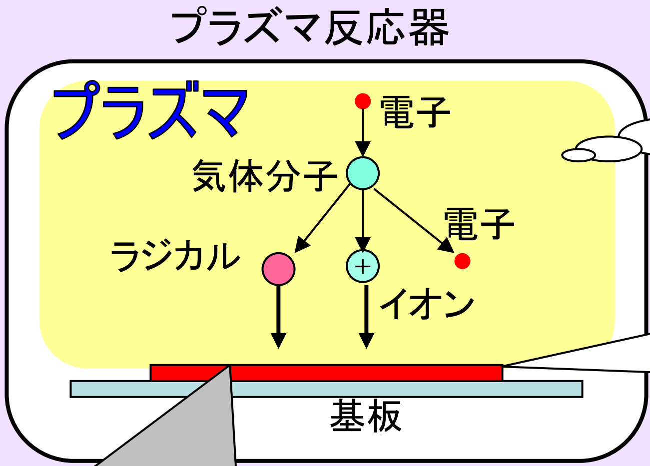
M+, M*, M- → Fragmentation

→ Radicals, Ions

(Reactive plasma)

Controlling materials at molecular levels

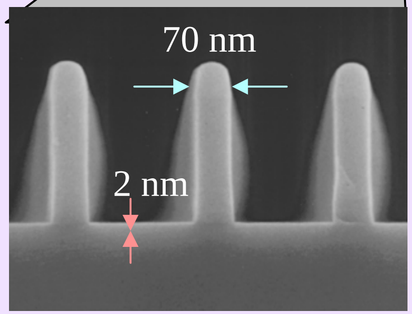
プラズマを用いた薄膜の堆積・加工



プラズマ中の
電子ー分子衝突によって
活性種が作られる

・薄膜を積む
・薄膜をけずる
・表面を改質する

拡大図



プラズマの利点： 低温で大量生産

LSI製造工程の50%にプラズマを使用

しかし，**プラズマは制御が困難**

⇩

活かせ **プラズマの可能性**

材料診斷－PIXE

- PIXE- Particle Induced X-ray Emission

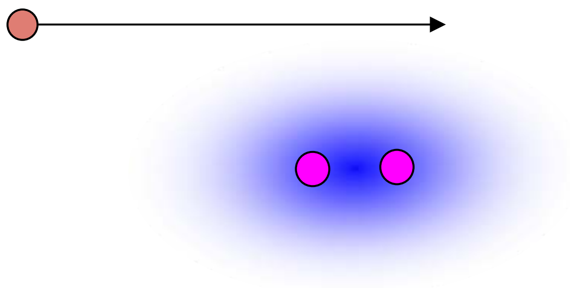
Basic Numbers in Atomic world

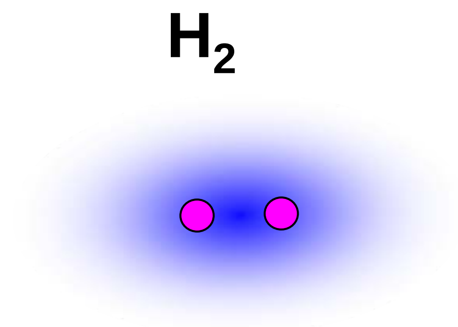
- **Size of atoms**:
  - **H(1): 0.529 x 10^{-8} cm**
  - **Fe(26): 1.34 x 10^{-8} cm**
  - **U(92): 2.32 x 10^{-8} cm**
- **Size of molecules**
  - **H2: 0.741 x 10^{-8} cm**
  - **N2: 1.10 x 10^{-8} cm**

An order of the size of atoms and molecules: ~10^{-8} cm

- **Mass**
  - **electron: 9.11 x 10^{-28} g**
  - **proton: 1.67 x 10^{-24} g**
- **Energy**
  - **H ionization energy: 13.6 eV**
  - **H2 molecule dissociation energy: 4.48 eV**
- **Velocity**
  - **H(1s) orbital velocity: 2.19 x 10^{8} cm/s**
  - **Velocity of light: 2.998 x 10^{10} cm/s**
  - **O2 gas in 27C: 4.2 x 10^{4} cm/s**

Atomic scales





Collision time

$>10^{-16}$ s for keV

Vibrational period

$< 10^{-13}$ s

Time scales

$T_{elec} = 0.01$ fs

$T_{vib} = 15$ fs

Energies

$I_p = 16$ eV

$E_{vib} = 0.5$ eV

$D_e = 4.75$ eV

Length scales

$R_e = 0.74 \times 10^{-8}$ cm

History of Atomic Collision Research

1911 Rutherford and Geiger
α-particle on thin film—Atom model

1914 Franck and Hertz
Electron beam—Discrete energy

-1930 Ramsaur and Townsend,
Electron-Rare gas collisions–
Lighting, Discharge,….

Born, Bethe, Massey,…….
Rydberg, Auger,…….

1945 Synchrotron, Accelerator,…
1970 Laser, Ion sources,…

1980- Explosion!

Development of Quantum Mechanics

Atomic energy, Space Science Fusion, Medical, High-Tech.,…

- **Number of atoms and molecules**

1 cm^3 中:　　~10^{23}個　　固体

2.7×10^{19}個　　常温1気圧気体

10-10000個　　星間空間

原子衝突の研究の歴史

1911　Rutherford and Geiger　　α粒子－金薄膜衝突による原子モデルの確立

1914　Franck and Hertz　　電子線による原子の離散エネルギーの発見

~1930　Ramsaur and Townsend　　放電による希ガス衝突

Rydberg, Born, Bethe, Massey-Mott, Auger,…..
量子力学の創設と完成に大いに貢献

~1945以降

シンクロトロン、加速器、レーザー、核融合、医療………..
近代技術発展に多大な貢献

Collisions processes

- **Ion impact**

$A^+ + B \rightarrow A + B$ **Elastic** **no threshold**

Inelastic

$\rightarrow A^+ + B^+ + e$ **Ionization** **~10eV**

$\rightarrow A + B^+$ **Charge transfer** **~ eV**

$\rightarrow A^+ + B^*$ **Excitation**

(Electronic, Ro-vibrational)

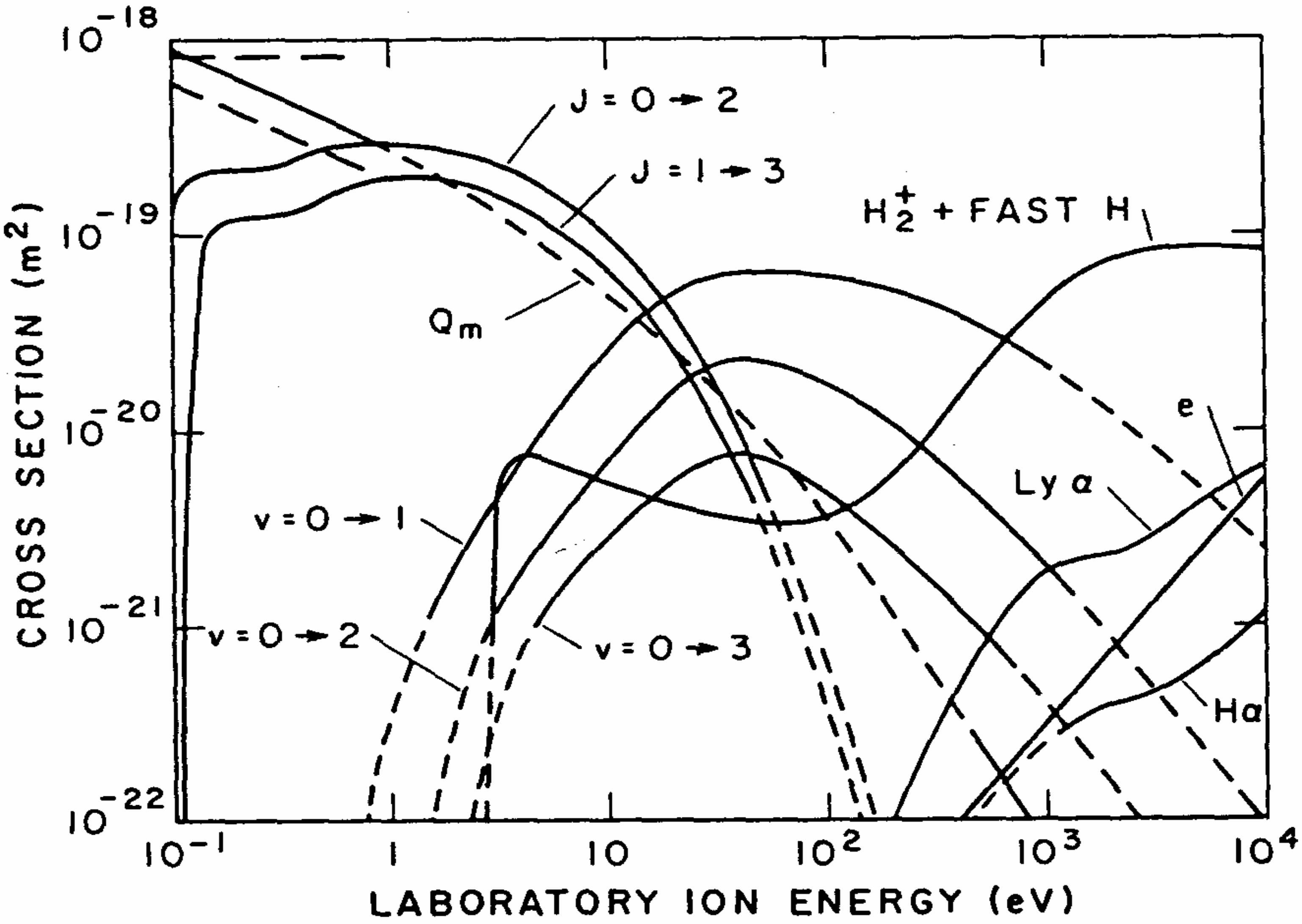
~meV - ~10eV

$\rightarrow C + D$ **Reactive** **~meV**

- **Electron impact**

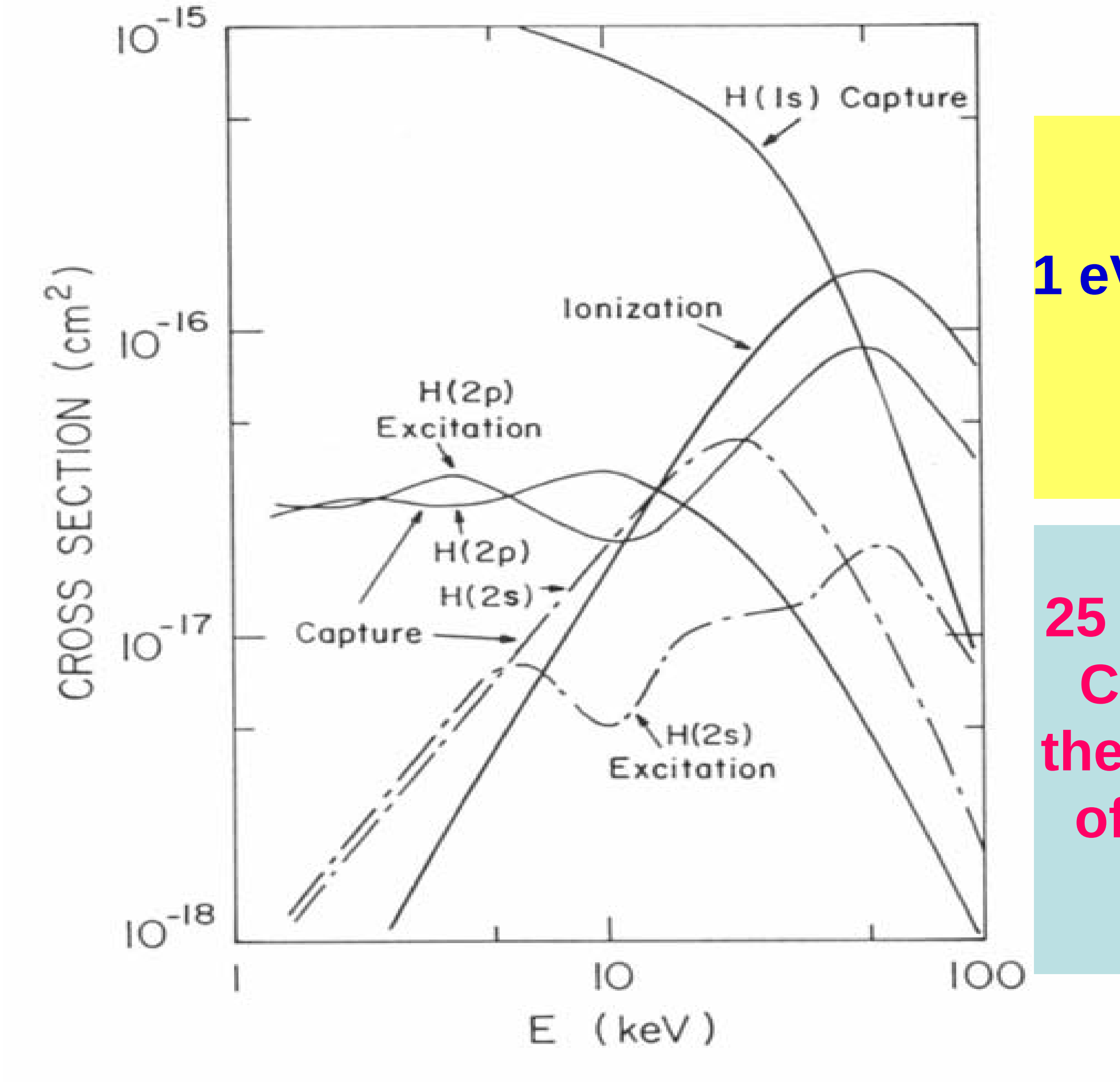
- $e + M \rightarrow M^{-*} \rightarrow A + B^-$ **Dissociative Electron Attachment (DEA)**

$H^+ + H_2$ Collisions:
Which processes are possible and how large are they?



H^+ + H Collisions

: which processes are important in what degree ?

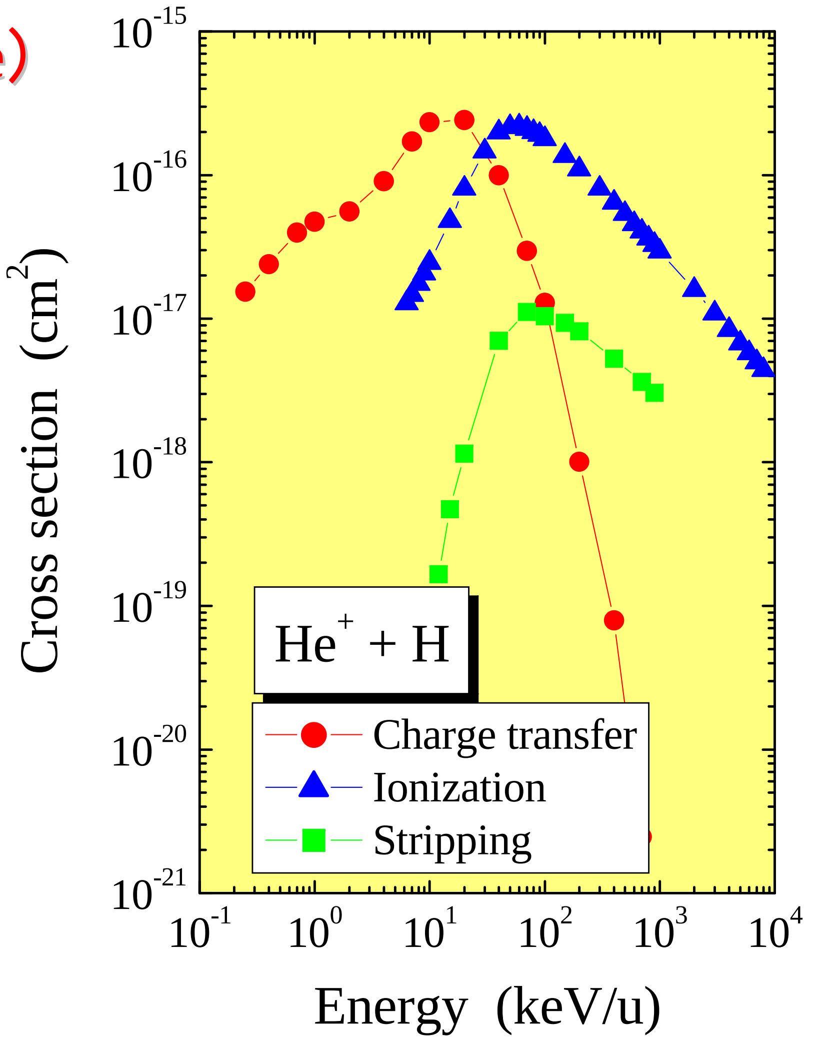


Energy :
1 eV = 23.1 kcal/mol
= 11000 K
= 8070 cm^{-1}

25 keV for H+ ions Corresponds to the orbital velocity of H(1s) electron

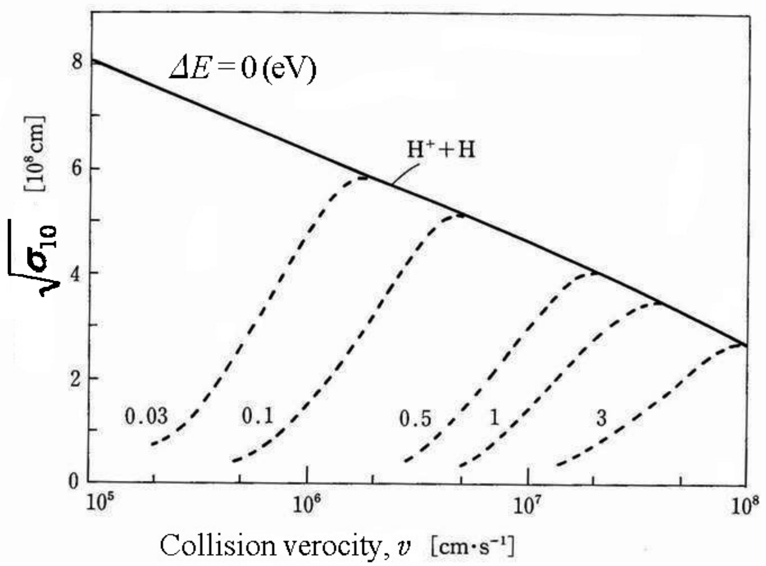
Representative collision processes
ex. $He^+ + H$ collisions

- **Charge transfer: (electron capture)**
  $He^+ + H \rightarrow He + H^+$
- **Ionization: (of target particles)**
  $He^+ + H \rightarrow He^+ + H^+ + e^-$
- **Stripping: (electron loss; ionization of projectile ions)**
  $He^+ + H \rightarrow He^{2+} + H + e^-$
- **Charge transfer → dominant in low collision energy region**
- **Ionization and Stripping → dominant in relatively high collision energy region**



Resonant charge transfer process

Atomic target B: $A^+ + B \rightarrow A^0 + B^+ + \Delta E \quad (\Delta E = I_A - I_B)$



D. Rapp and W. E. Francis, *J. Chem. Phys.*, **37**, 2631 (1962)

I_A, I_B : Ionization potential

ΔE : Energy defect

$\Delta E < 0$: endothermic

$\Delta E > 0$: exothermic

$\Delta E = 0$: Resonant charge transfer

$$\sigma_{RES} \sim (a - b \cdot \log v)^2$$

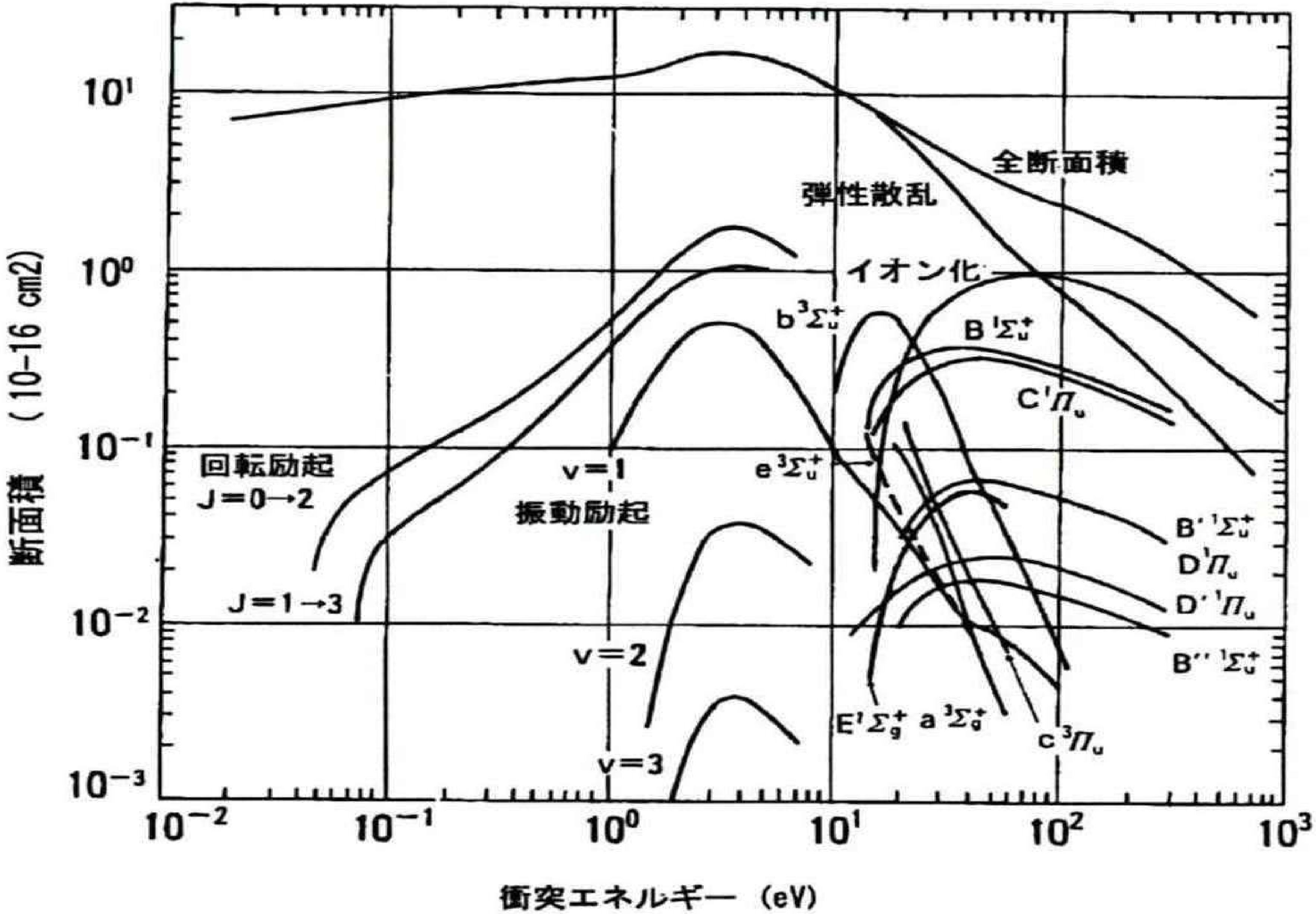
Molecular target M:

$$A^+ + M \rightarrow A^0 + M^+(n_v) + \Delta E$$

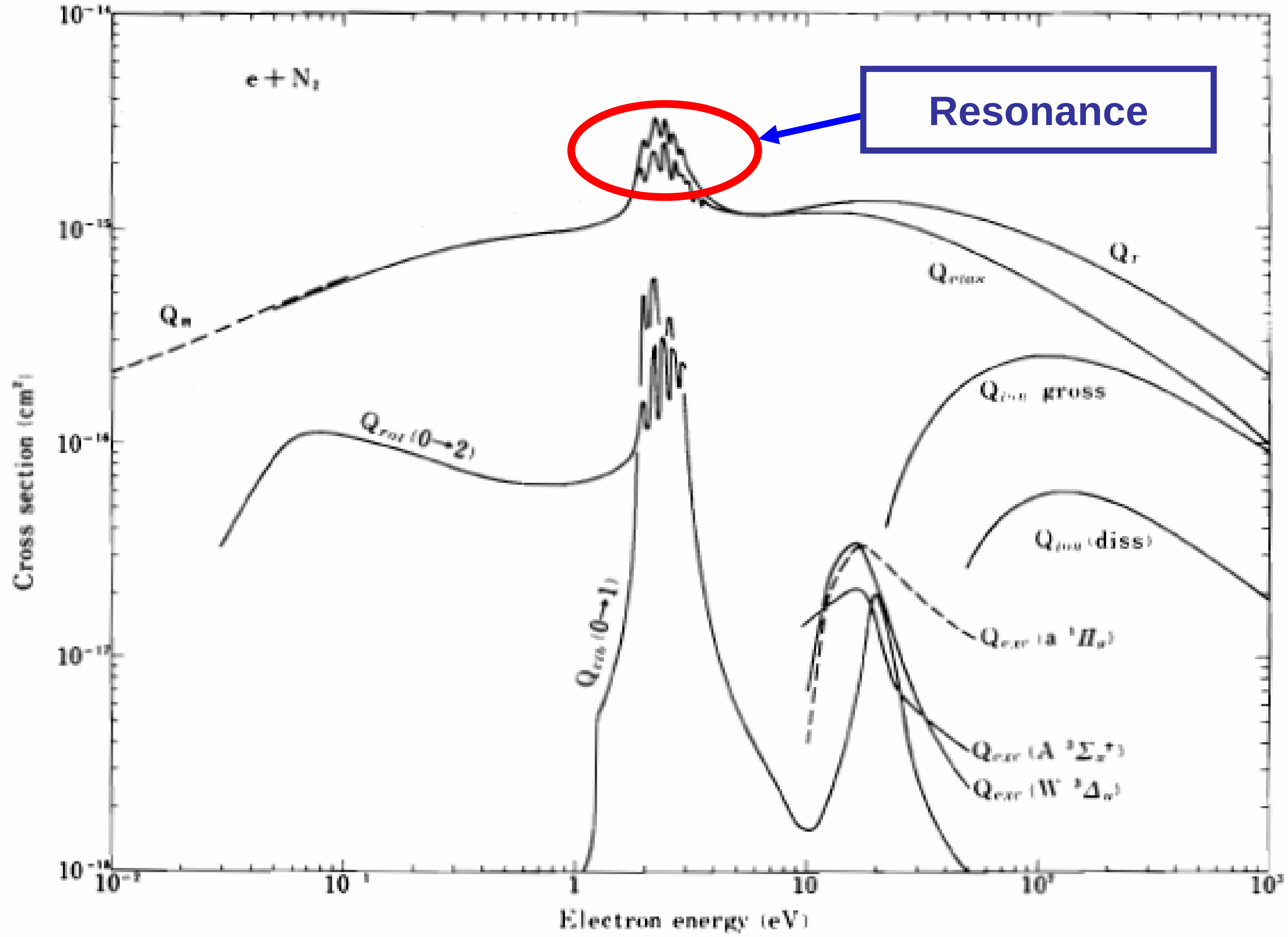
$$\Delta E = (I_A - [\, I_M + E\,(n_v)\,])$$

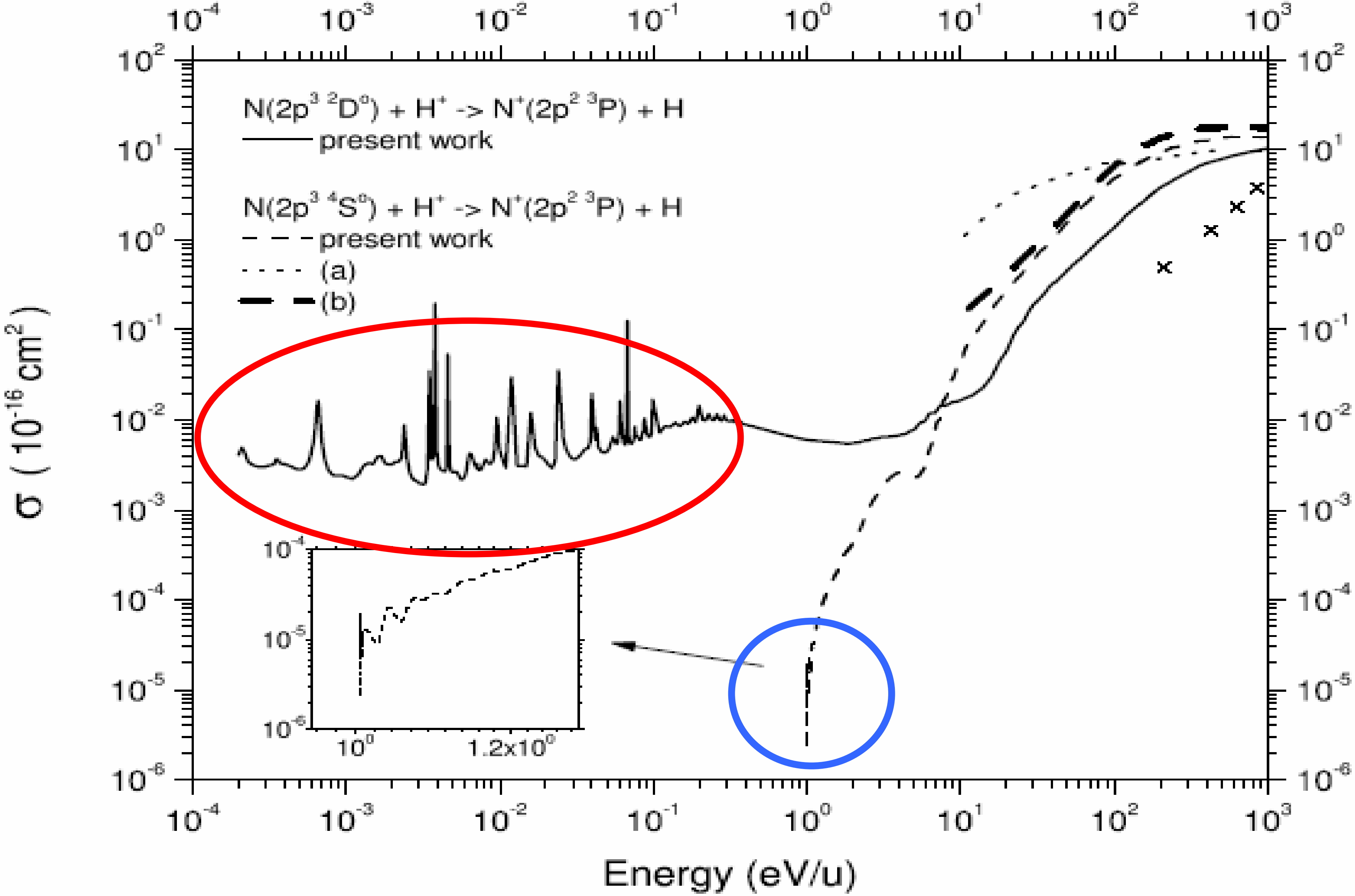
If $I_A > I_M$, the excess energy can be spent on making the vibrational excited states of the product molecular ions, and this results in creation of near or accidental resonant charge transfer channels.

e + H2 collisions



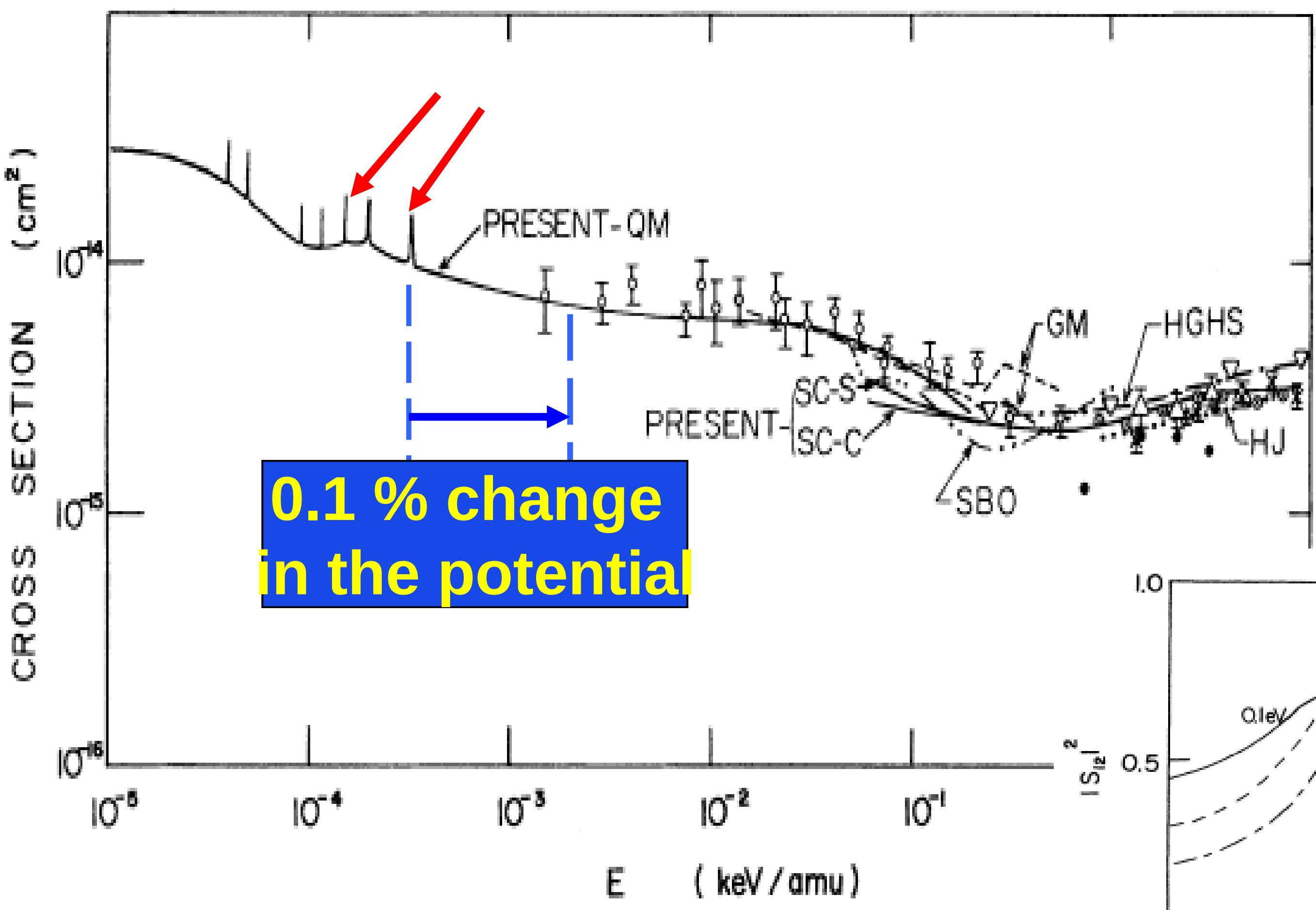
e + N2 collisions

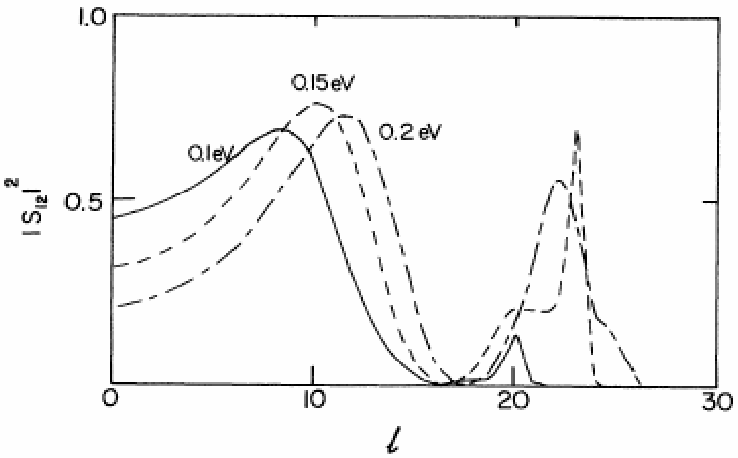




N(2p3 2Do) + H+ -> N+(2p2 3P) + H
present work
N(2p3 4So) + H+ -> N+(2p2 3P) + H
present work
(a)
(b)
σ (10-16 cm2)
Energy (eV/u)
1.2x100

Charge transfer cross sections





PHYSICAL REVIEW A VOLUME 44, NUMBER 3 1 AUGUST 1991

Electron capture in collisions of N^{5+} ions with H atoms from the meV to keV energy regions

N. Shimakura* and M. Kimura
Argonne National Laboratory, Argonne, Illinois 60439
and Department of Physics, Rice University, Houston, Texas 77251

Resonances

- Shape resonance

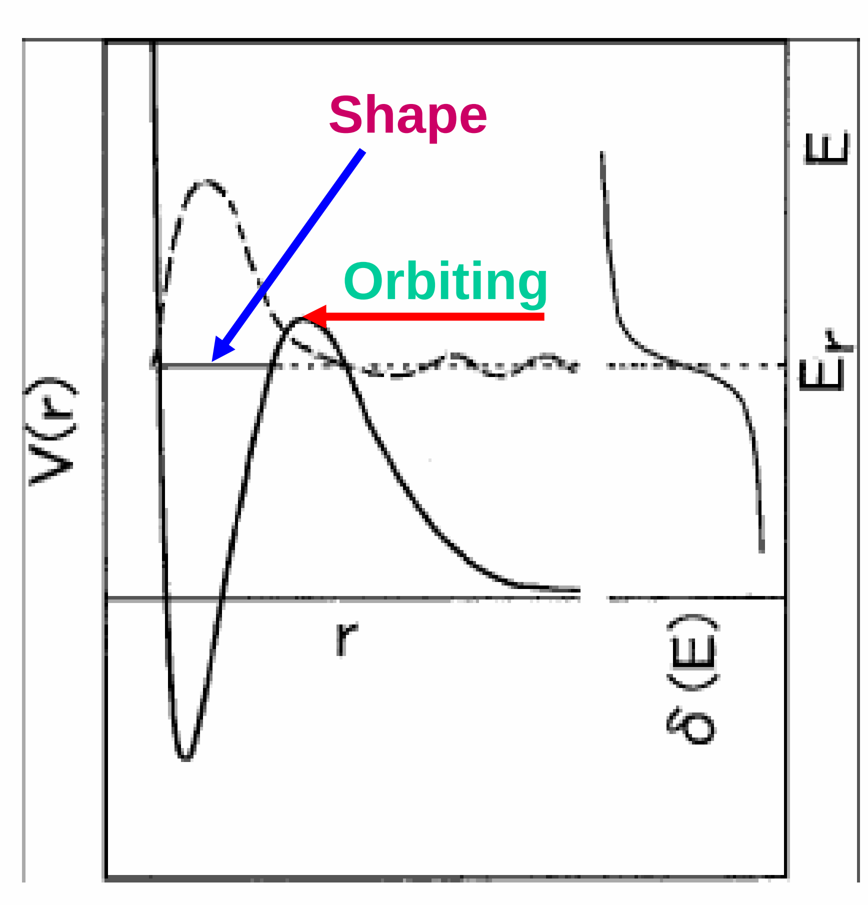
  1つのポテンシャル面

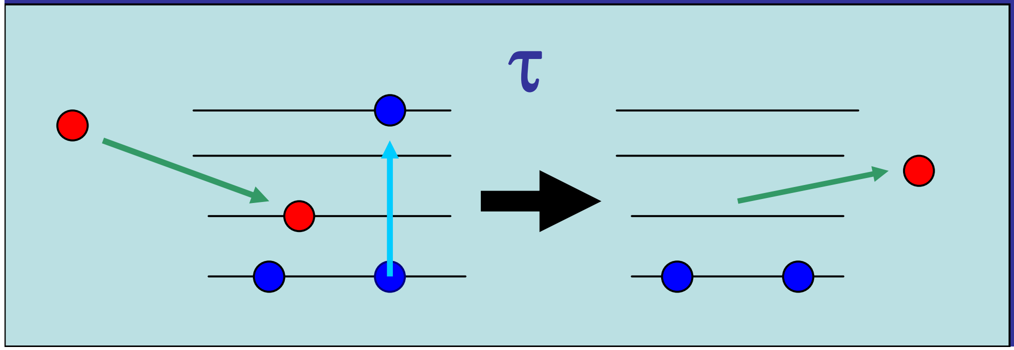
- Orbiting resonance

  1つのポテンシャル面

- Feshbach resonance

  内部状態の励起が関与





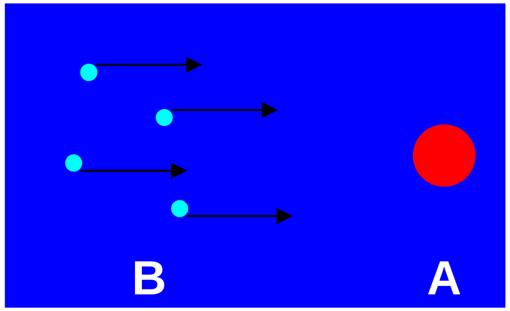
Conversion of energy unit

- 1 eV = 1.602 x 10^{-19} J = 96.49 kJ/mol = 23.06 kcal/mol = 8065.7 cm^{-1}
- 1eV = 電子eを1ボルトの電位差で加速したときに電子が得るエネルギー

Basic of Atomic Collisions

- **Cross section**

BとAが衝突する頻度*f*は、飛んでくる粒子の量に比例。1cm^{2}の断面を単位時間当たり*j*個の原子Bが通過すると、



$$f = \sigma x j$$

ここでσは断面積の次元を持つ物理量である。

入射粒子Bにとっては、標的粒子Aの断面積以内に入れば必ず衝突し、そこからはずれれば衝突しない。このσを「衝突有効断面積」と呼ぶ。

ここで全粒子Bは同じ速度*v* cm/s持つとし、1cm^{3}中にn_B個あるとすると　$j = n_B \times v$

∴　$f = n_B v \sigma$

*f*を衝突頻度(Collision frequency)と呼ぶ。

また、

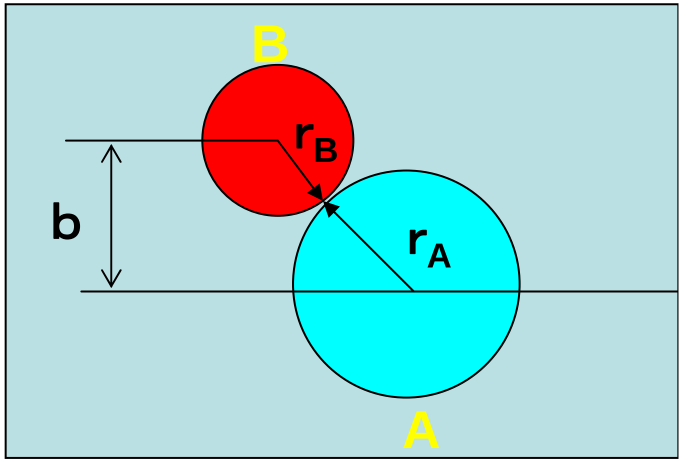
$z = \sigma v$

を衝突頻度因子(Collision frequency factor)と呼ぶ場合があるが、これは分子反応の反応し易さを表す反応定数に他ならない。

- **More of Cross Sections**

剛体球の衝突を考える。粒子A,Bの衝突で2つの球は $b \leq (r_A + r_B)$なら必ず衝突する。粒子AとBが衝突するこの場合の衝突有効断面積は

$$\sigma = \pi (r_A + r_B)$$



ここで原子分子のおおよその大きさは10^{-8}cm程度であるのでその断面積の大きさはおおよそ10^{-16} cm^2が目安と考えられる。

- **Note:**

剛体球の場合、粒子の境界がはっきりしているが、原子分子の場合、境界ははっきりしておらず、原子分子の電子雲の広がりによる。従って、断面積の決定は原子分子1つずつ、又飛んでくる入射粒子ごとに、決める必要がある。一般に衝突断面積の大きさは10^{-14} cm^2-10^{-17} cm^2

非弾性散乱断面積の場合

$$\sigma^{ile} = \sigma^{tot} \times p$$

p：ある非弾性散乱過程が起きる確率。

弾性散乱の場合の断面積と少し意味が異なっていることに注意。

- **Experimentally determination of cross sections**

$$I_{out} = I_{in} exp(-\sigma \ell n_B)$$

where I_{out}, I_{in} are the final and initial beam intensities, respectively, ℓ is the length of the collision chamber, n_B the gas density, and σ cross section. By measureing I_{out}, I_{in} , σ can be determined.

- **Total cross sections**

$$\sigma^{tot}(E) = \Sigma_i\, \sigma_i(E) = \sigma_{el} + \sigma_{ion} + \sigma_{exc} + \ldots..$$

断面積と他の物理量の関係

- 平均自由行程(Mean free path)

$$\lambda_m = \frac{1}{n_B \sigma}$$

→ 電気伝導度、……

- 拡散係数(Diffusion coefficient)

$$D = \frac{v\lambda}{3}$$

→ミクローマクロを繋ぐ量

熱伝導、電気伝導、

古典的な粒子の衝突を考える

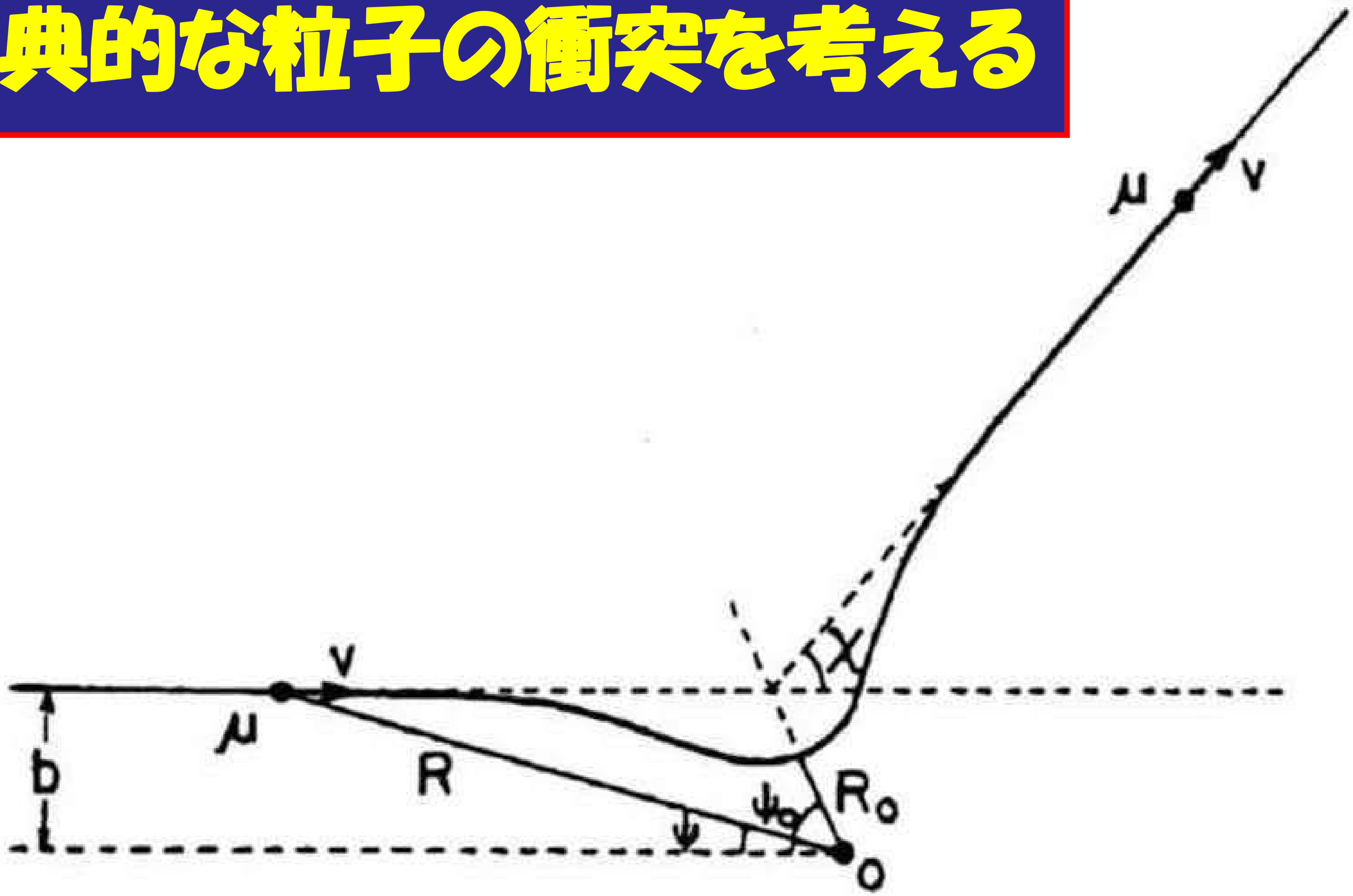


図 2.2.5　入射粒子と標的粒子との座標系

古典論による散乱

- 中心力場による散乱

散乱された粒子の散乱角θは衝突係数bと衝突エネルギーEの関数として:散乱関数

$$\Theta(b,E) = \pi - 2\int_{r_0}^{\infty} \frac{b}{\sqrt{1-\frac{b^2}{r^2}-\frac{V(r)}{E}}}\frac{dr}{r^2}$$

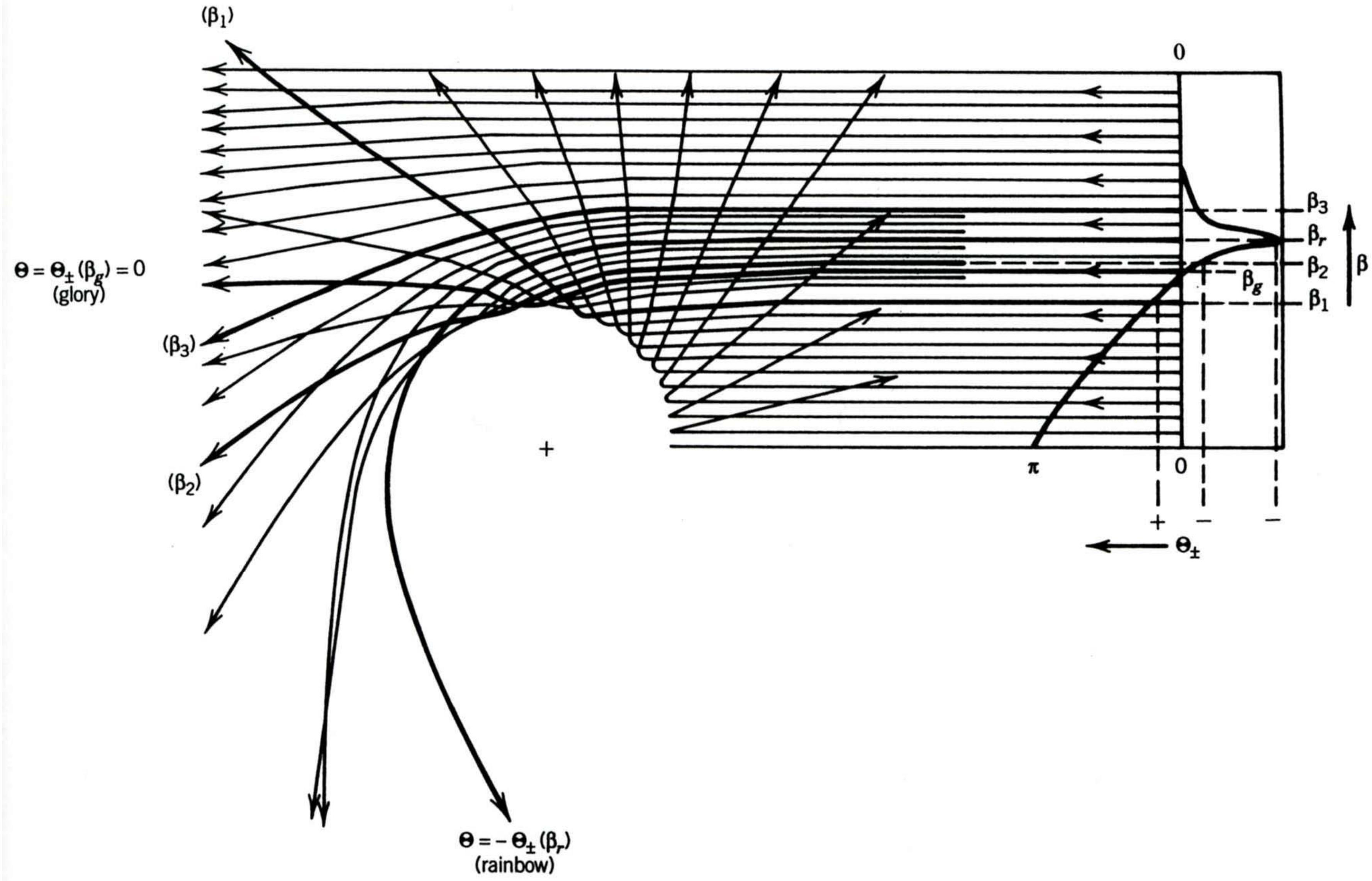
微分散乱断面積$d\sigma/d\Omega$は

$$\frac{d\sigma(E,\theta)}{d\Omega} = \frac{1}{\sin\theta}\sum_i b_i \left| \frac{1}{\left(\frac{d\Theta}{db}\right)} \right|_{b_i}$$

断面積の発散

異なるbから干渉が現れる

断面積と相互作用ポテンシャルの関係



(β1)
0
β3
βr
β2
βg
β1
β
Θ = Θ± (βg) = 0
(glory)
(β3)
(β2)
+
π
0
+
−
−
Θ±
Θ = − Θ± (βr)
(rainbow)

- $d\theta/db=0$ で微分断面積は発散

  → レインボウ（虹）散乱

- $\sin\theta = 0$ で微分断面積は発散

  → グローリー散乱

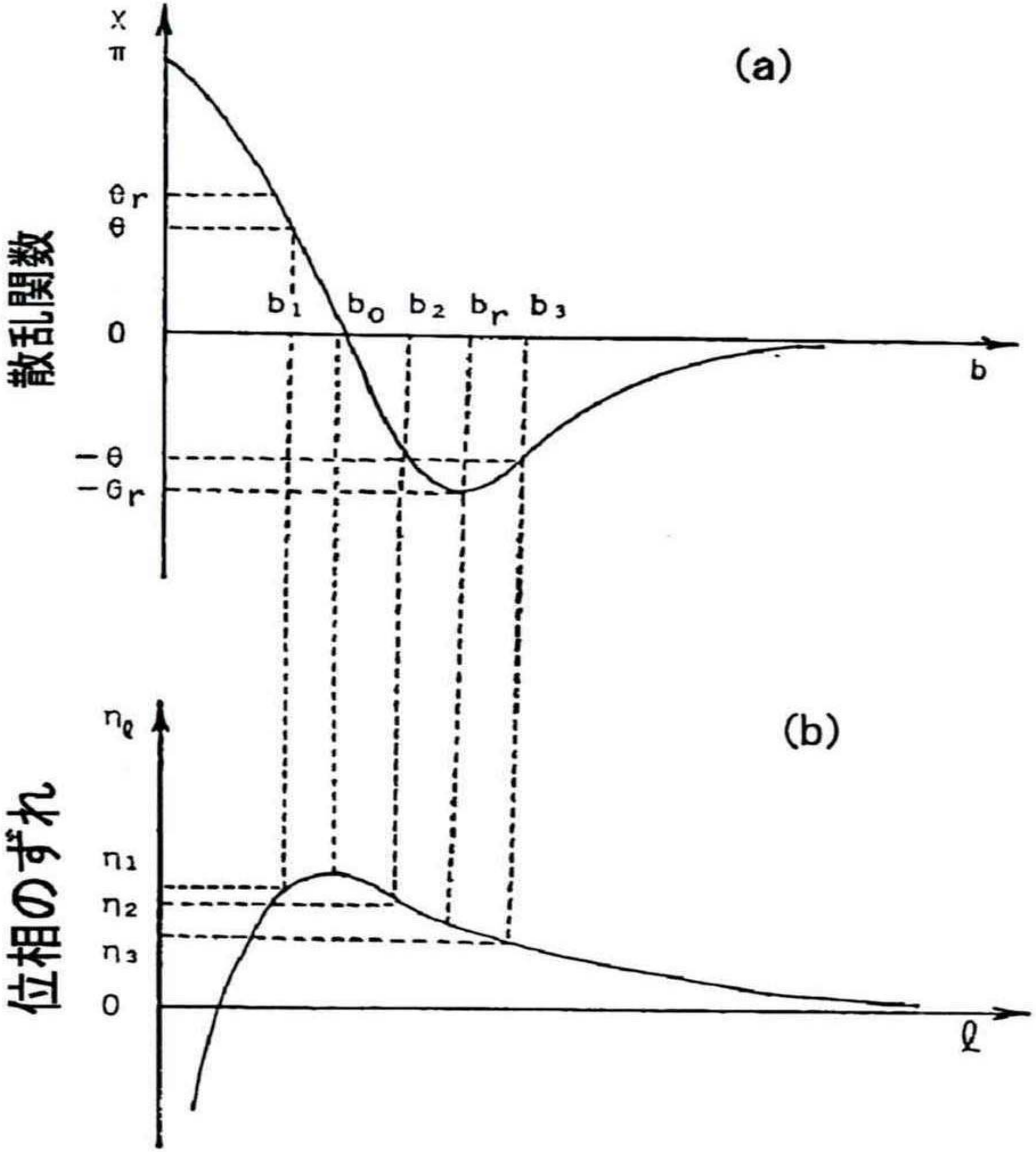


図 2.2.7　散乱関数と位相のずれと衝突係数との関係

散乱関数と位相のずれの関係

散乱関数と
相互作用ポテンシャルV(r)
との関係

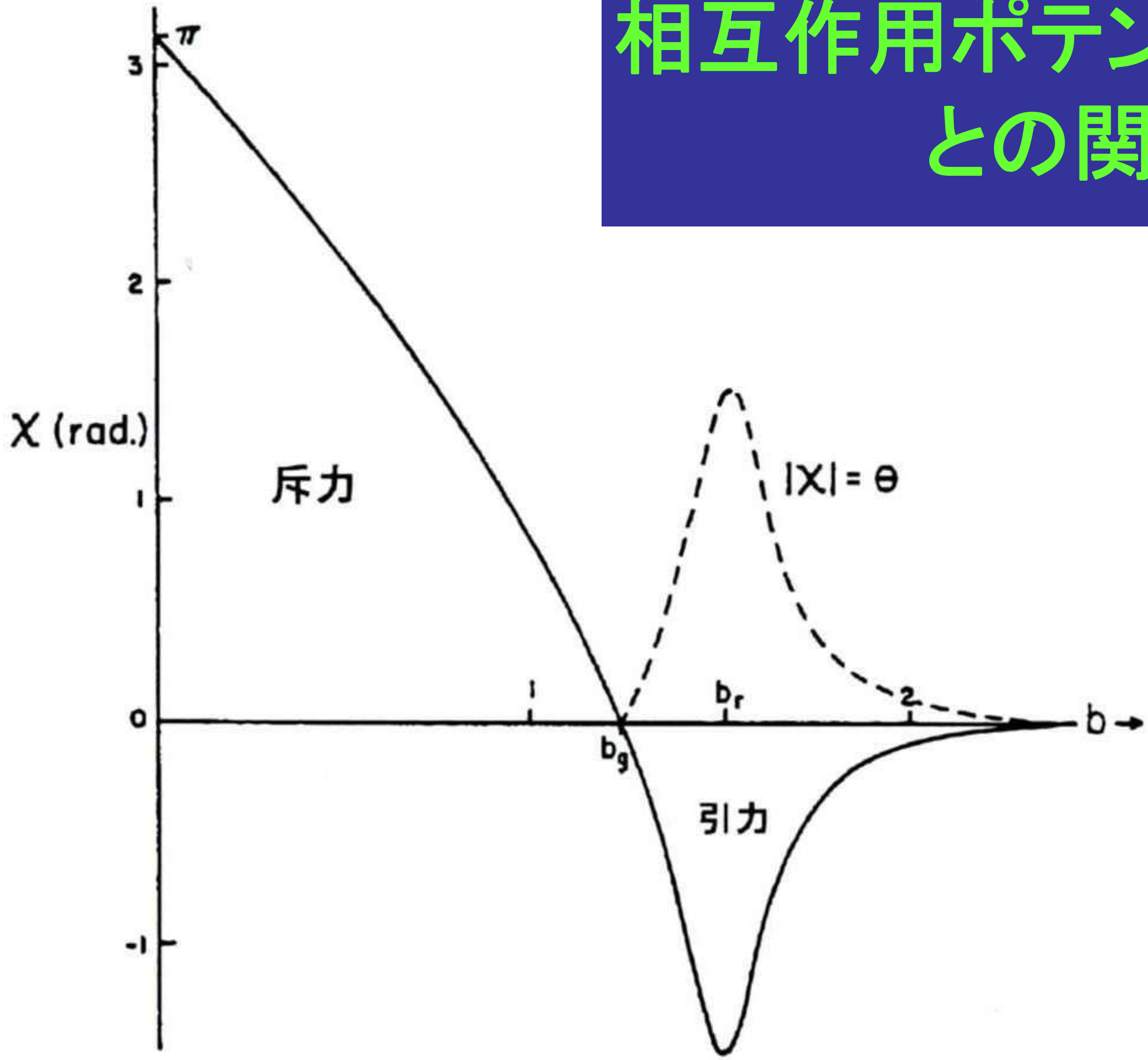


図 2.2.6　散乱関数とポテンシャルとの関連

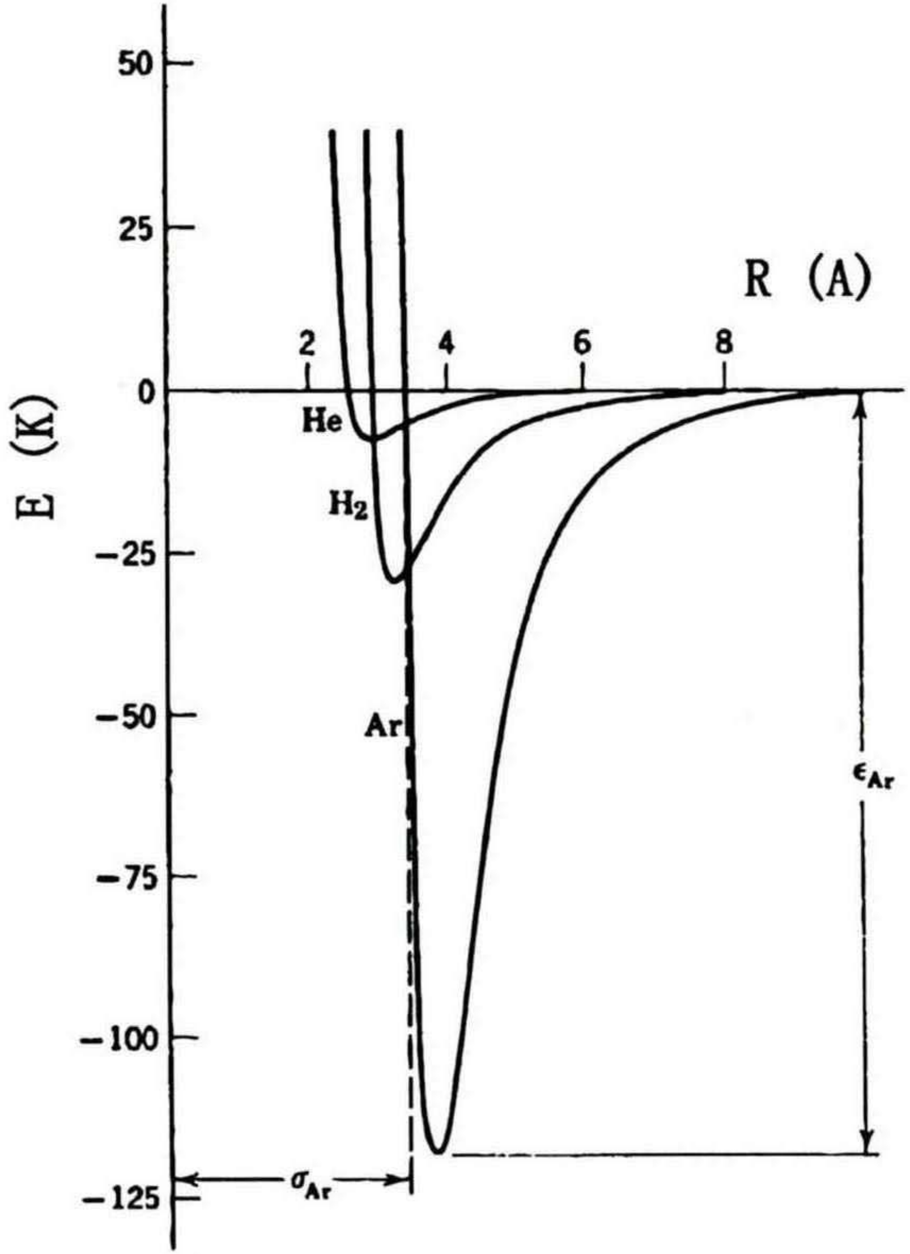
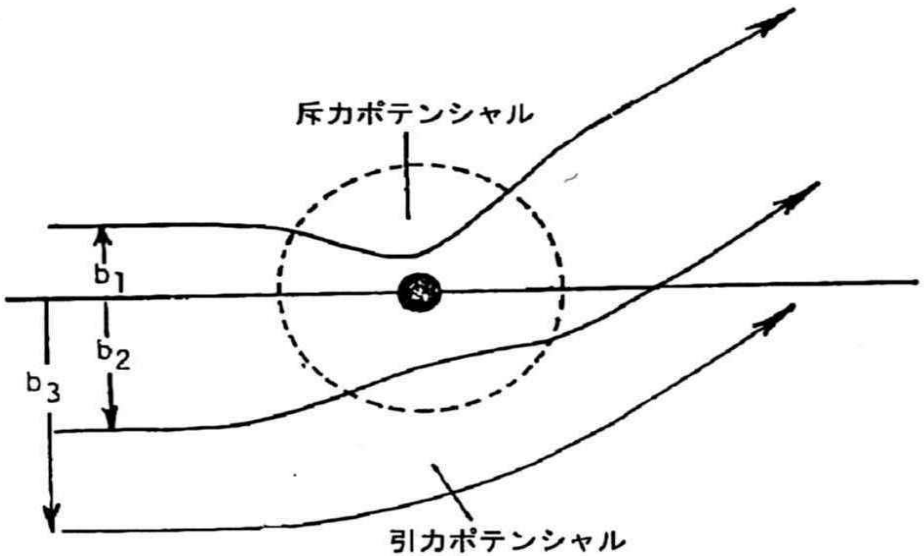


図 2.2.8　Lenard-Jones ポテンシャルの例

一般的な
相互作用ポテンシャル
———

Lenard-Jones (LJ)
Potential
基底状態のみ
（実験値+計算値から
製造）



相互作用ポテンシャル
と
レインボウ散乱
の関係

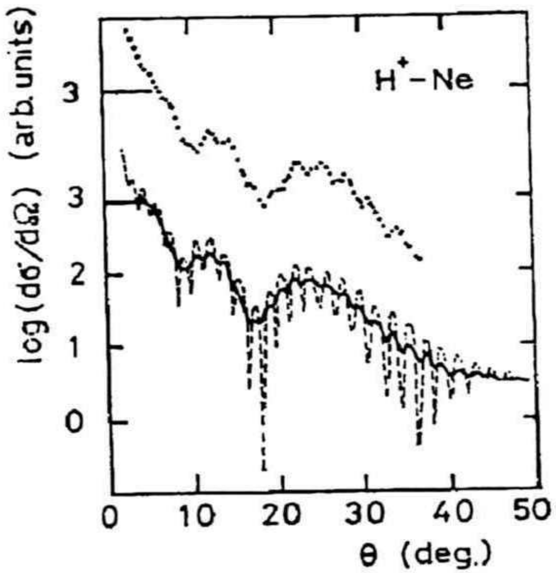


図 2.2.10　レインボー散乱とレインボー散乱の実験値例

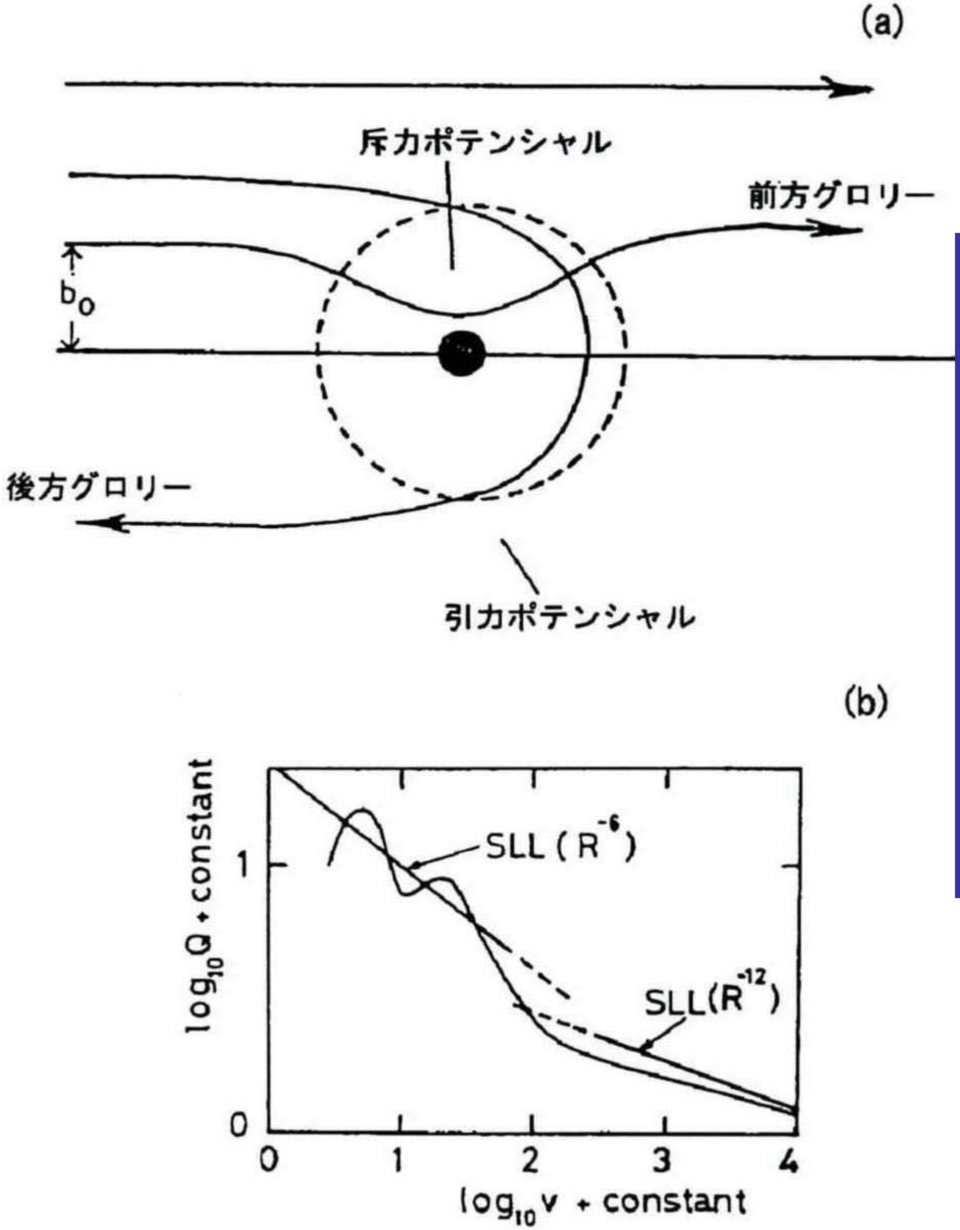
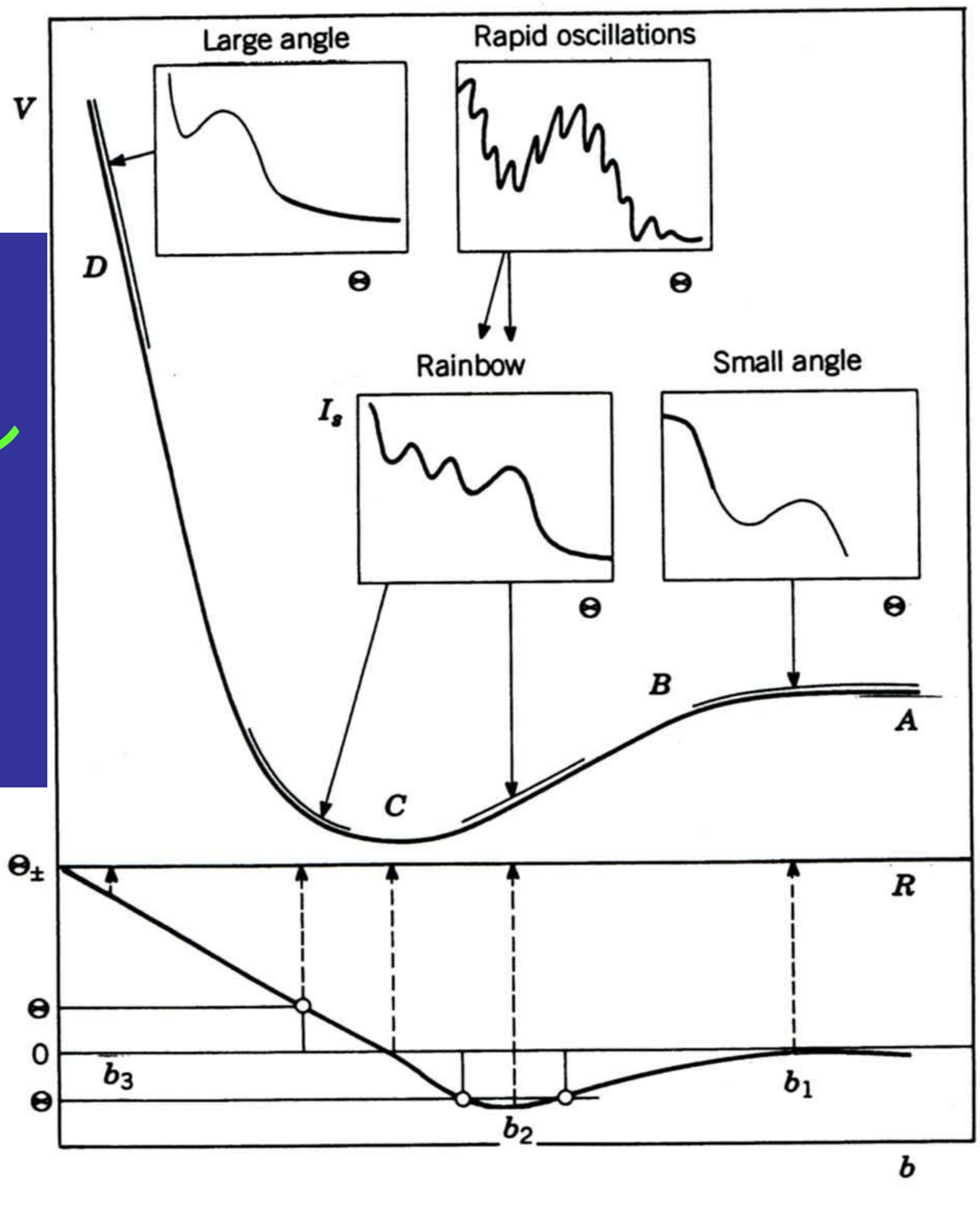


図 2.2.9　グロリー散乱と全断面積

相互作用ポテンシャル と グローリー散乱の関係

相互作用ポテンシャルV(r)と散乱関数との関係



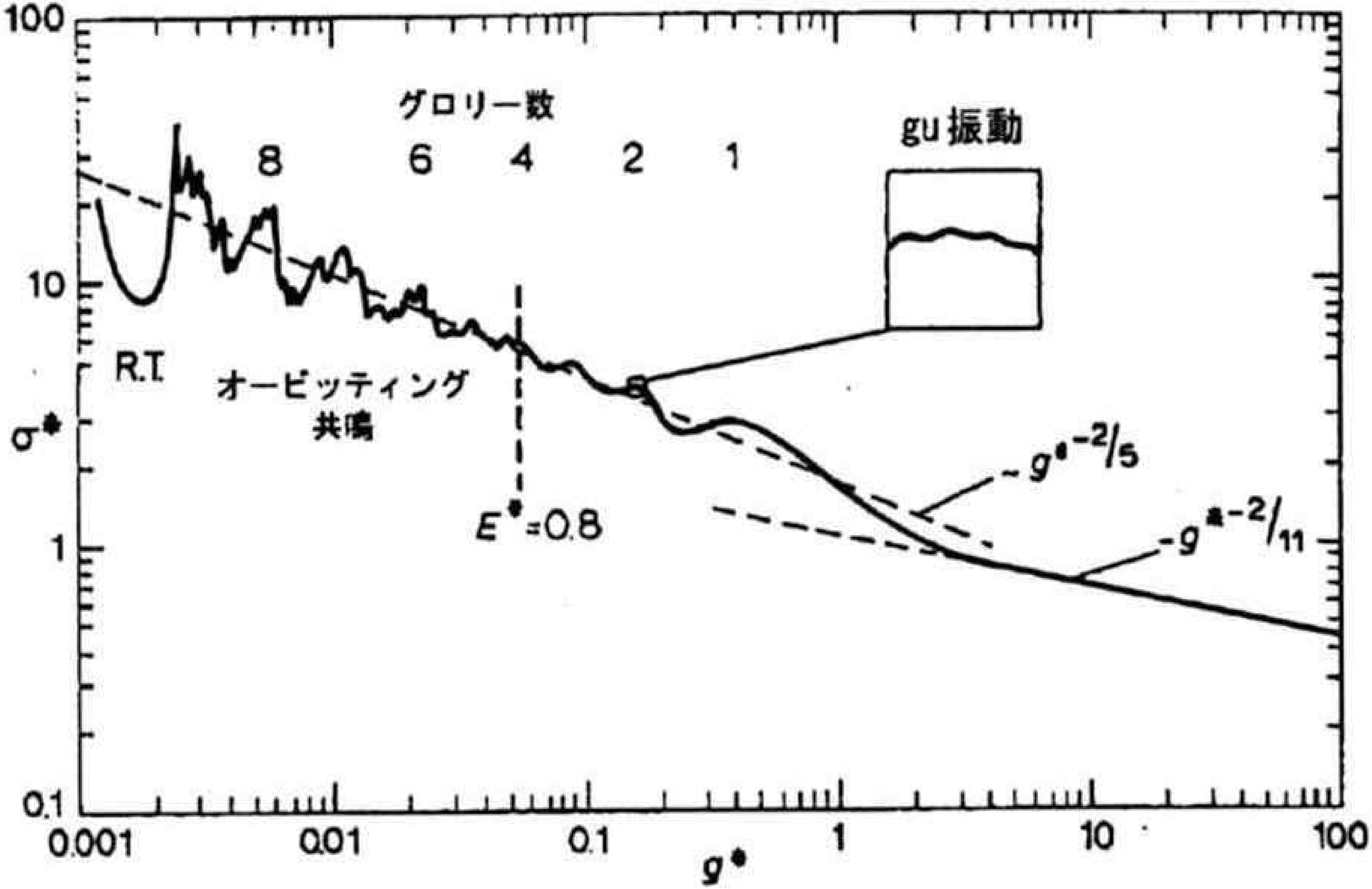


図 **2.2.13** LJ ポテンシャルでの弾性散乱計算例

量子論による衝突論

- Schrödinger equation for the [e^- + p]

$$\nabla^2\Psi + \frac{2m}{\hbar^2}\{E - V(r)\}\Psi = 0$$

(i) Bound state

$$\Psi \to \underline{Ce^{-\alpha r}} \text{ at } r \to \infty$$

減衰波

- E : Negative value

(ii) Continuum state

$$\Psi \to +\underline{Ce^{ikz}} + \underline{f(\theta,\varphi)\frac{e^{ikr}}{r}} \text{ at } r \to \infty$$

入射波　散乱波

E: Positive value

where $f(\theta, \varphi)$ is the scattering amplitude.

- **Differential cross sections**

$$\frac{d\sigma(\theta,\varphi)}{d\Omega} = \left|f(\theta,\varphi)\right|^2$$

- **Total cross sections**

$$\sigma(E) = \int_0^{4\pi} \left|f(\theta,\varphi)\right|^2 d\Omega = \int_0^{4\pi} \frac{d\sigma(\theta,\varphi)}{d\Omega} d\Omega$$

$f(\theta, \varphi)$ の求め方

- 入射波

$$\phi_{in} = e^{ikz} = \sum_{l=0}^{\infty}(2l+1)i^l P_l(\cos\theta)\frac{\sin(kr - l\pi/2)}{kr}$$

- 散乱波

$$\phi_{scatt} = \phi - \phi_{in} = \sum_{l=0}^{\infty}\frac{e^{ikr}}{2ikr}(2l+1)(e^{2i\eta_l} - 1)P_l(\cos\theta)$$

η_l:位相差

- 散乱振幅

$$f(\theta) = \frac{1}{2ik}\sum_{l=0}^{\infty}(2l+1)(e^{2i\eta_l} - 1)P_l(\cos\theta)$$

- Scattering S-matrix

$$S = e^{2i\eta}$$

断面積

- 一般的な断面積の式

$$\sigma(E) = \frac{4\pi}{k^2} \sum_{l-0}^{\infty} (2l+1) \sin^2 \eta_l$$

- 部分波についての和と*sin*関数のために様々な構造が断面積に現れる。
- →共鳴、干渉、多体効果、…….

量子論：共鳴構造の例

- 対称2状態（例：水素原子ー水素原子）

$$\sigma(E) \propto \sum_l (2l+1)\sin^2[\eta_g(l)-\eta_u(l)]$$

$$\Delta\eta \propto \int_b^\infty \frac{[V_g(R)-V_u(R)]}{(1-\frac{b^2}{R^2})^{1/2}} dR$$

- 断面積はポテンシャルの差に依存

断面積の構造

- **弾性散乱（Single channel)**

  Ramsauer-Townsend effect

  Rainbow

  Glory

  Symmetry

- **共鳴**

  形状共鳴(Shape resonance:ポテンシャル共鳴)

  オービッティング共鳴(Orbiting resonance)

- **非弾性散乱 (Multi-channel)**

- **共鳴**

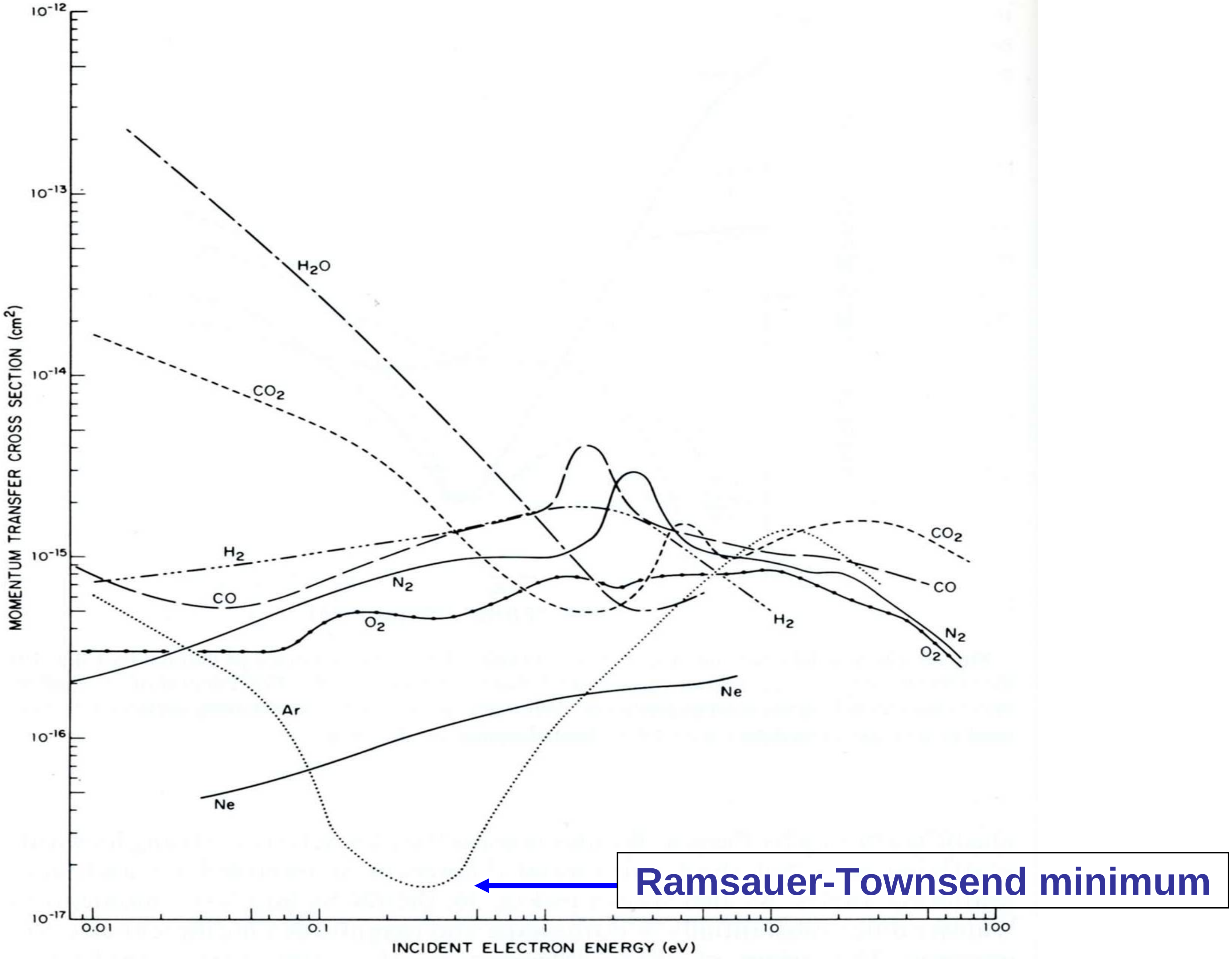
  フェッシュバッハ共鳴(Feshbach resonance)

- **干渉**

  反応道筋(Stückelberg,Rosenthal,…,Multi-channel)

- **多体効果**

  Post-collision interaction, Shake-off, ….



MOMENTUM TRANSFER CROSS SECTION (cm²)
10⁻¹²
10⁻¹³
10⁻¹⁴
10⁻¹⁵
10⁻¹⁶
10⁻¹⁷
0.01
0.1
1
10
100
INCIDENT ELECTRON ENERGY (eV)
H₂O
CO₂
H₂
CO
N₂
O₂
Ar
Ne
CO₂
CO
H₂
N₂
O₂
Ne
Ramsauer-Townsend minimum

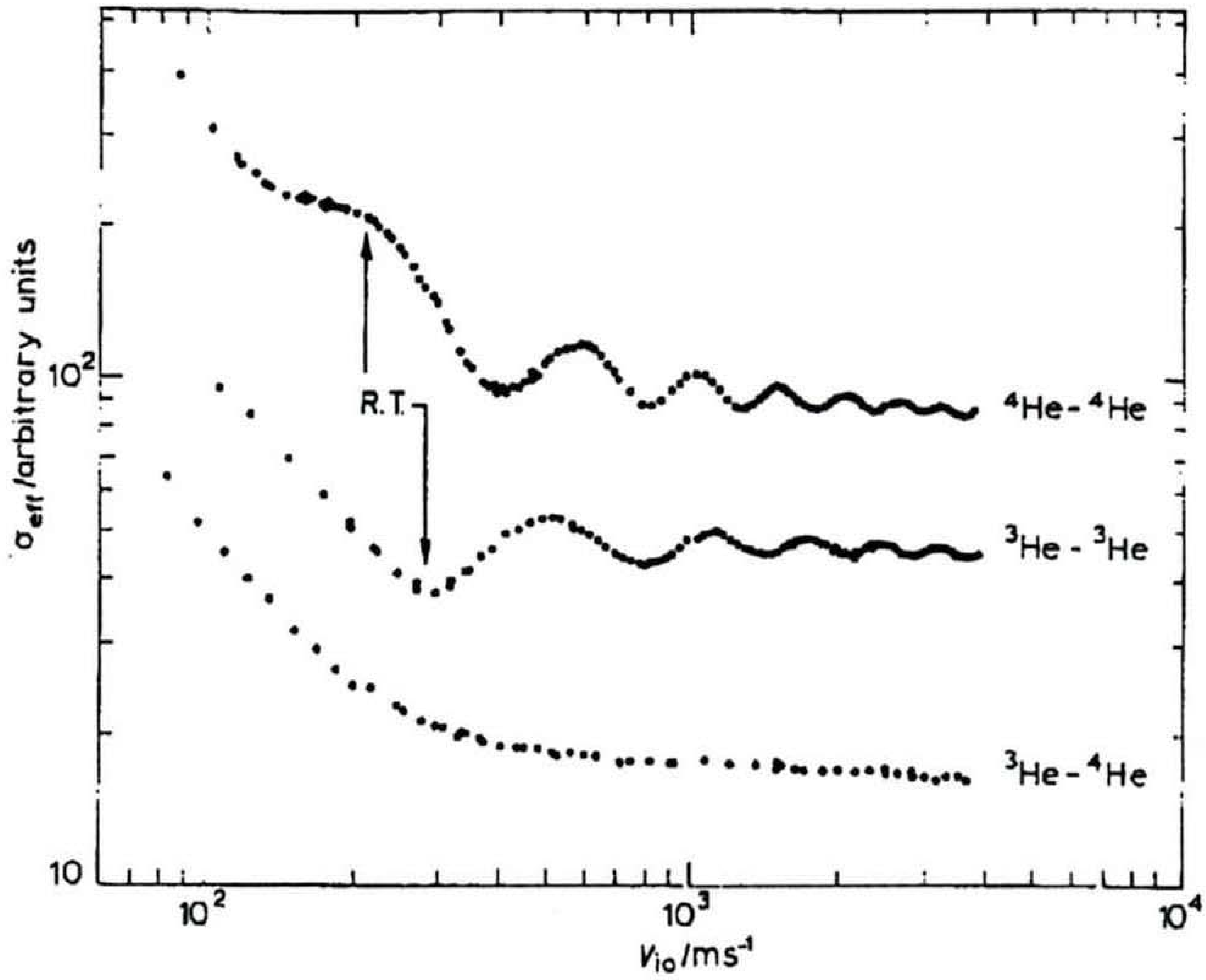


図 2.2.11 He-He 衝突による gu 振動。同じ質量の粒子間の衝突の時のみ振動が表れる。

近似的な断面積：Born近似

- Born近似による断面積

  (a) 相互作用が弱い.

  (b) 入射波、散乱波のゆがみは小さい。

- 電子と原子の衝突を考える。

$H_a(r_a)$*:** 原子のハミルトニアン、$V(r_a, r)$*:** 電子ー原子　相互作用

$$\{-\frac{\hbar^2}{2m}\nabla_r^{\;2} + H_a(r_a) + V(r_a, r) - E\}\psi(r_a, r) = 0$$

$$\psi(r_a, r) = \sum_m F_m(r)\varphi_m(r_a)$$

$$H_a(r_a)\varphi_a(r_a) = \varepsilon_a \varphi_a(r_a)$$

Schrodinger eq.を書き換える。

$$(\nabla^2 + k_a{}^2)F_a(r) = \sum_\beta U_{\alpha\beta}(r)F_\beta(r)$$

$$U_{\alpha\beta}(r) = \frac{2m}{\hbar^2}\int \varphi_f{}^*(r_a)V(r_a, r)\varphi_a(r_a)dr_a$$

相互作用が小さいとし、右辺＝0とおき、S. eqを解く

$$F^0{}_a(r) = \delta_{a0}\exp(ik_0 r)$$

$F^0{}_a(r)$を代入すると

$$(\nabla^2 + k_a{}^2)F_\alpha{}^1(r) = U_{\alpha 0}(r)\exp(ik_0 r)$$

上式を解くと

$$F_{\alpha}^{1}(r) = -\frac{1}{4\pi}\int \frac{\exp\{ik_{\alpha}|r-r'|\}}{|r-r'|} U_{\alpha 0}(r')\exp(ik_0 r')dr'$$

散乱波、$\Psi \fallingdotseq \psi_{in} + (f(\theta, \phi)/r)\psi_{out} = F^0 + F^1$, より
散乱振幅が求まり

$$f(0\rightarrow\alpha;\theta,\phi) = -\frac{1}{4\pi}\int \exp\{i(k_0 - k_{\alpha})\cdot r'\} U_{\alpha 0}(r')dr'$$

入射波、散乱波　　標的原子の量

ExactなClosed coupling法

- 固有関数での全散乱波動関数の展開

$$\psi(\vec{r},R)=\sum_i X_i(R)\phi_i^{BO}(\vec{r},R)F_i$$

X(R): 核波動関数、$\phi(r, R)$:電子波動関数、
F(r):**Electron Transfer Factor (ETF)**

- Quantum mechanical coupled equation

$$\frac{1}{2\mu}\left\{-i\frac{\partial^2}{\partial R^2}+\left(\vec{P}+\vec{A}\right)\right\}^2+\vec{\varepsilon}(R)-E\vec{I}\ \ \vec{X}(R)=0$$

正確なClose-coupled equations

全散乱波動関数

$$\Psi(r,t) = \sum_n a_n(t)\varphi_n(r)e^{-iE_n t/\hbar}$$

半古典論によるCoupled equation

$$i\hbar\frac{da_n}{dt} = \sum_m V_{nm}(r)e^{i\Delta E_{nm}t/\hbar}a_m(t)$$

展開basisの波動関数を動選ぶか？

- If $V_{rel} >> v_{orb}$, then it is regarded that during collisions, colliding particles keep their atomic characters.

→**Atomic basis expansion**

- If $V_{rel} << v_{orb}$, then colliding particles are considered to form quasi-molecule during collisions.

→**Molecular basis expansion**

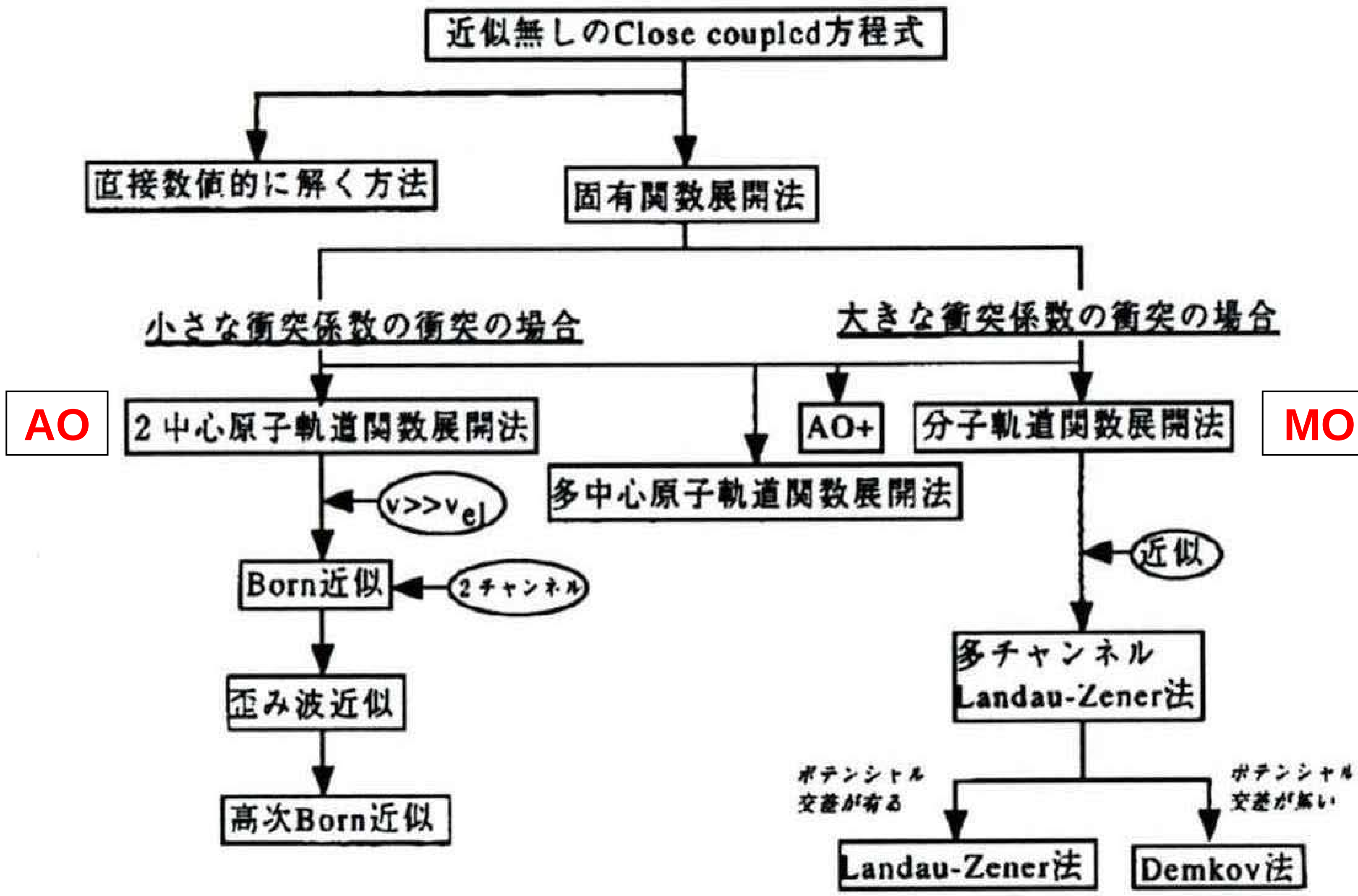


図 2.4.1　中間エネルギーで使われる理論モデル：緊密結合法と他の近似法との関係

Born seriesの収斂性

速度が十分高い場合、2項以降の寄与は小さく
第一項のみで十分断面積は収斂
→ First Born approx.

速度が遅くなるにつれ2項以降の項が寄与
→ Higher Born approx.

Lippamann-Schwinger eq.

$$\psi(r) = e^{ik_0 r} - \frac{2\mu}{\hbar^2}\frac{1}{4\pi}\int \frac{\exp(ik|r-r'|)}{|r-r'|}V(r')\psi(r')dr'$$

Vを摂動として波動関数を摂動展開し上式に代入

$$\psi = \psi^{(0)} + \psi^{(1)} + \psi^{(2)} + ...$$

両辺で同じ次数と等しいとおくと Born　展開式

$$\psi^{(0)} = e^{ik_0 r}$$

$$\psi^{(n)} = -\frac{2\mu}{\hbar^2}\frac{1}{4\pi}\int \frac{\exp(ik|r-r'|)}{|r-r'|}V(r')\psi^{(n-1)}(r')dr'$$

Born展開断面積

$$\sigma^{Born} = \sigma^{(1Born)} + \sigma^{(2Born)} + \sigma^{(3Born)} + \ldots\ldots\ldots$$

Born展開式が収斂するかどうかの保証はない。
充分高い衝突エネルギーでは第1次Bornで旨く記述できるが、衝突エネルギーが低くなるにつれ高次項が必要になってくる。高次項の計算は非常に厄介。

Born近似のまとめ

- 入射波、散乱波は平面波で近似。
- 相互作用は標的の波動関数にしかよらない。
- 2状態(channel)（初期状態、終状態）のみ考慮。

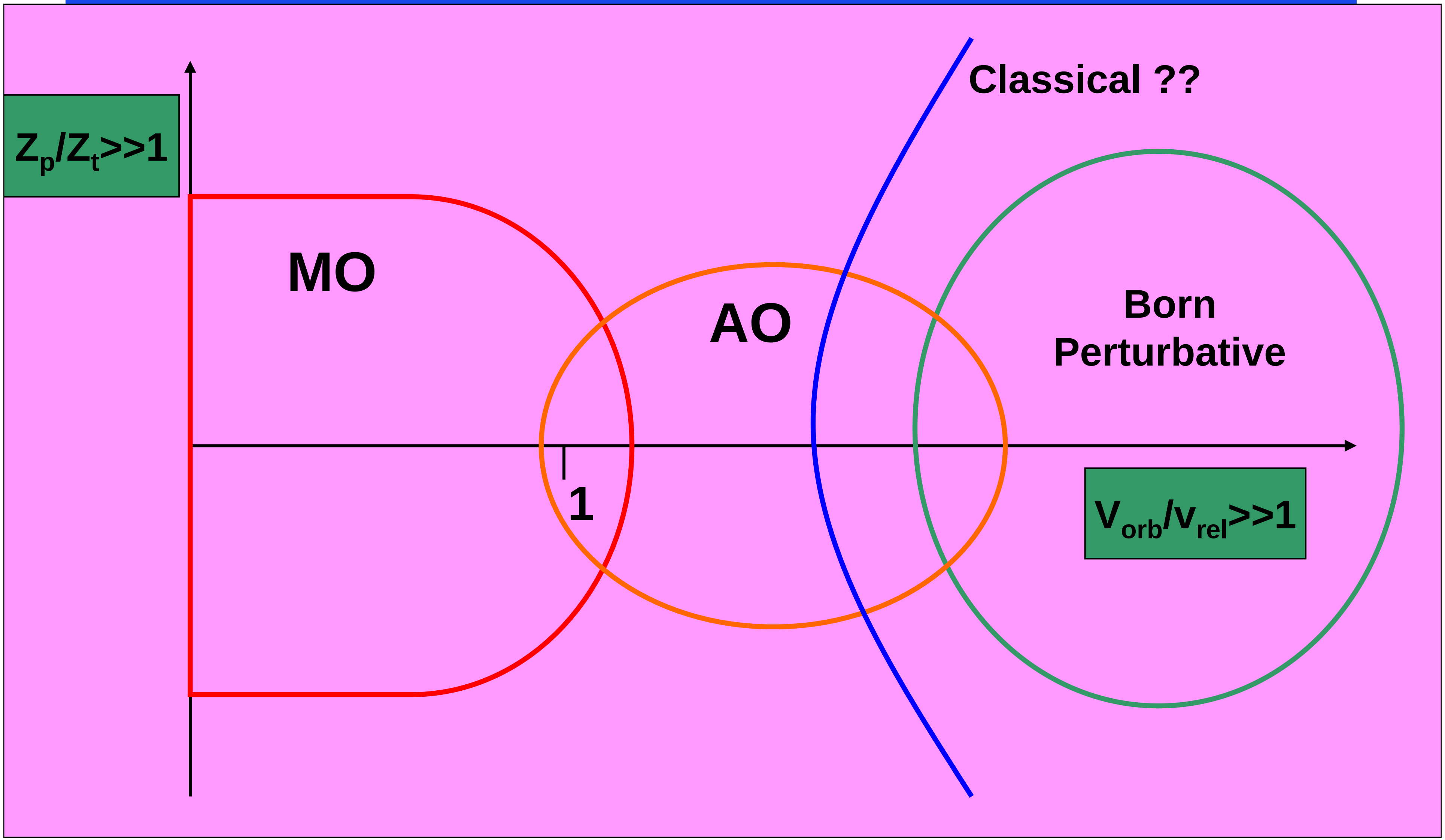
→高エネルギー衝突で遠距離衝突（相互作用時間が短く、相互作用が弱い）に成立。

→ 入射粒子に拠らない量になる。

Born まとめーつづき

- 十分高速での衝突では第一項で十分断面積は収斂—>1st Born approx.
- 速度が遅くなるにつれ高い項が必要になる。
- しかし、どのエネルギーで高い項が必要になるかはアプリオリには判らない。

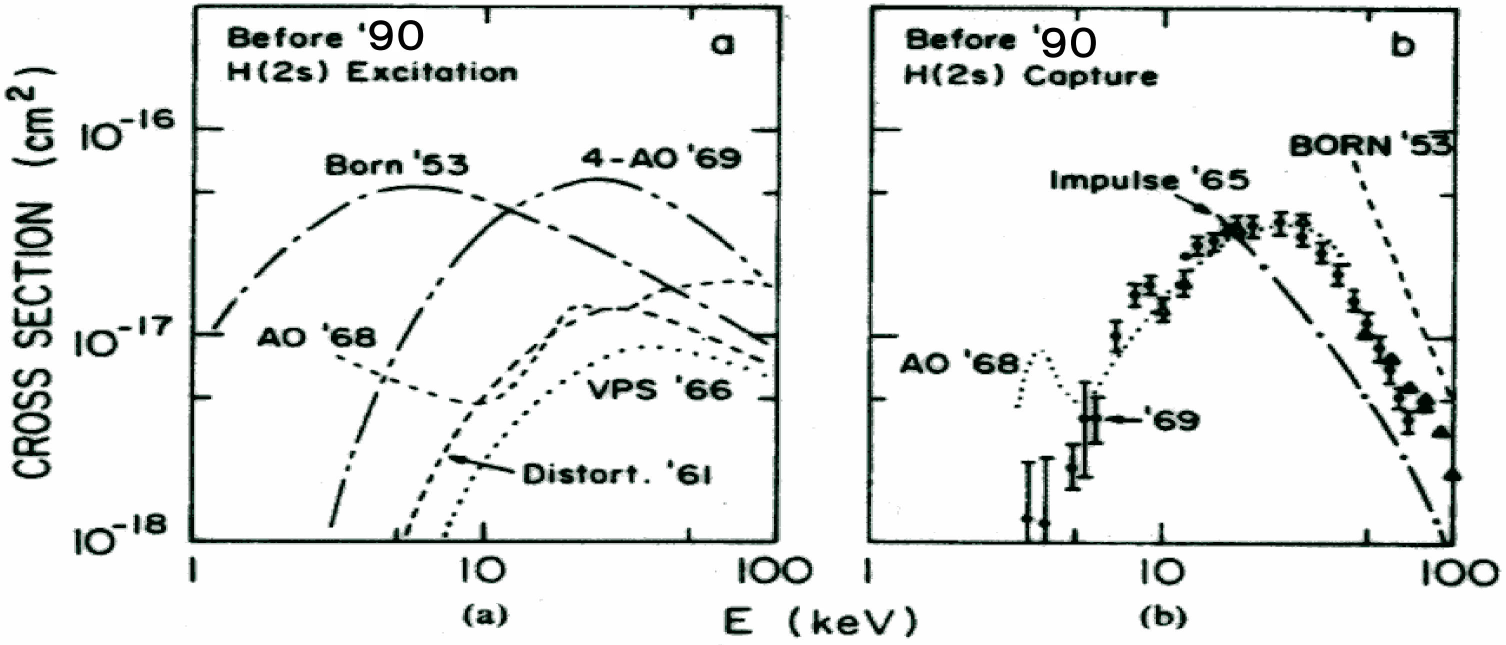
まとめ：
理論モデルの使える領域



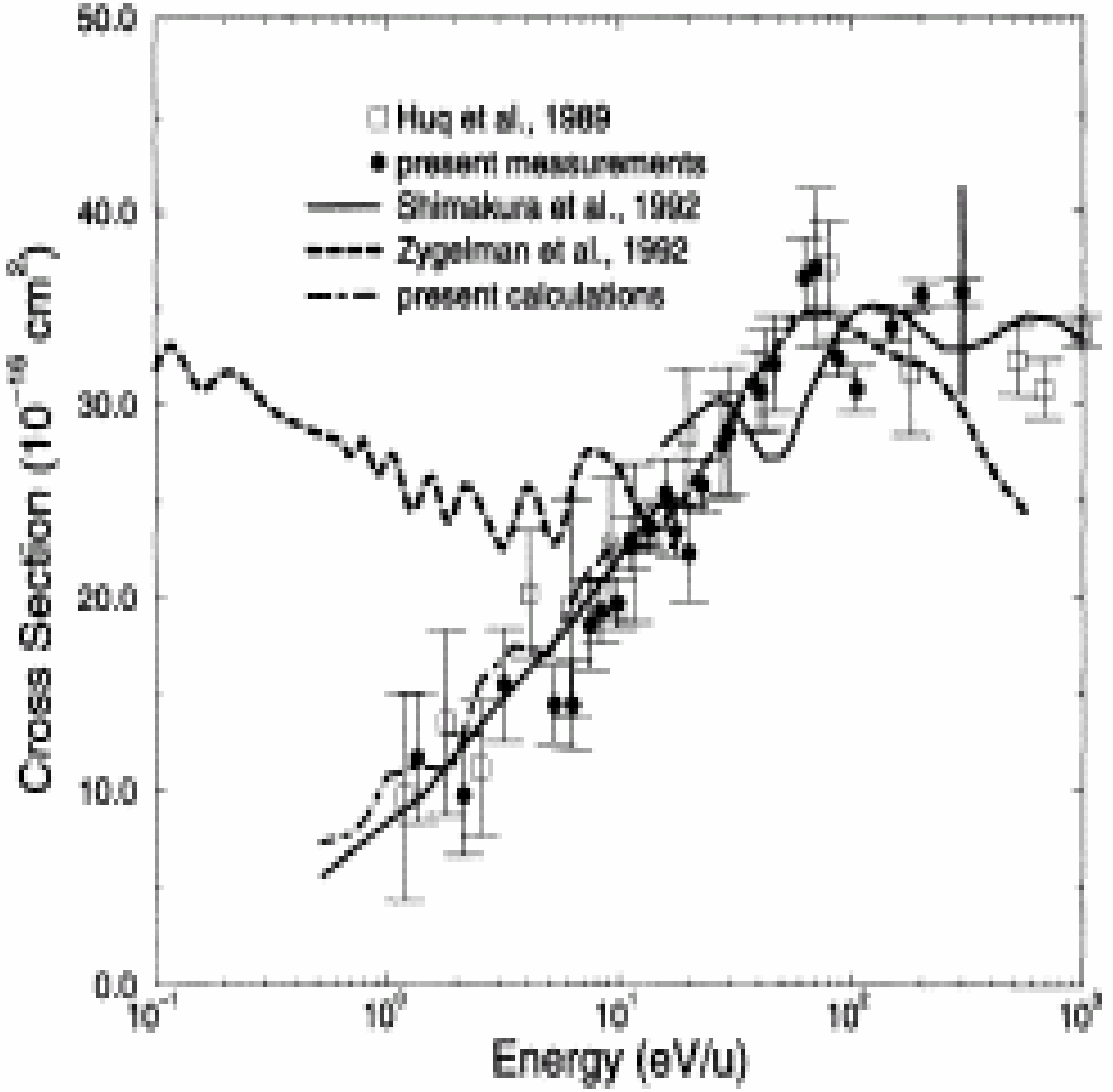
To Understand hydrogen is to understand all of physics.

Victor Weisskoph

Charge transfer in $H^+ + H \rightarrow H + H^+$ collisions

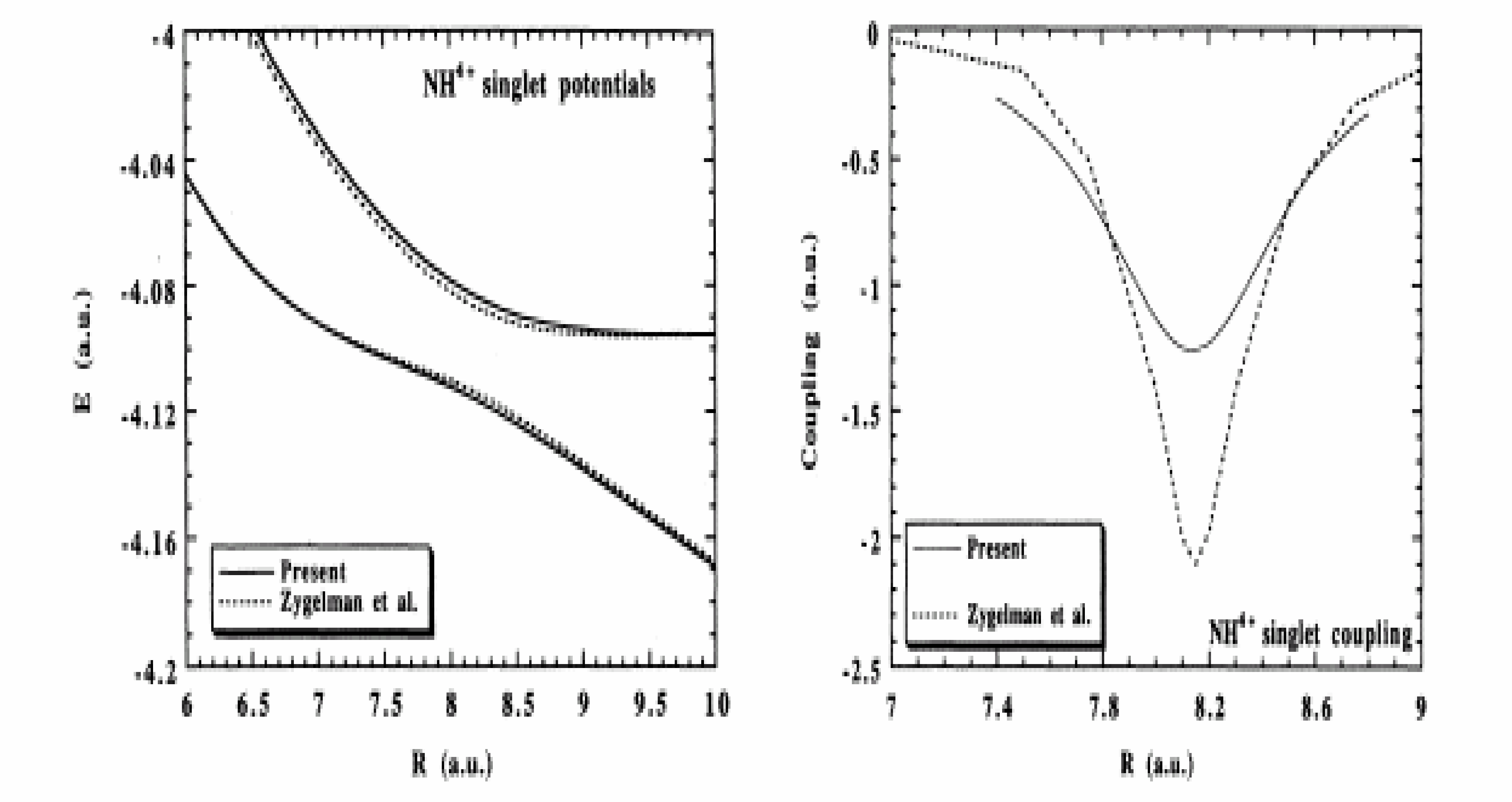


Charge Transfer in N^{4+} + H Collisions



Two sets of Theoretical results

Adiabatic potentials for the initial and final states, and the coupling



- $O^+(^4S) + H_2 \rightarrow O + H_2^+$ charge transfer

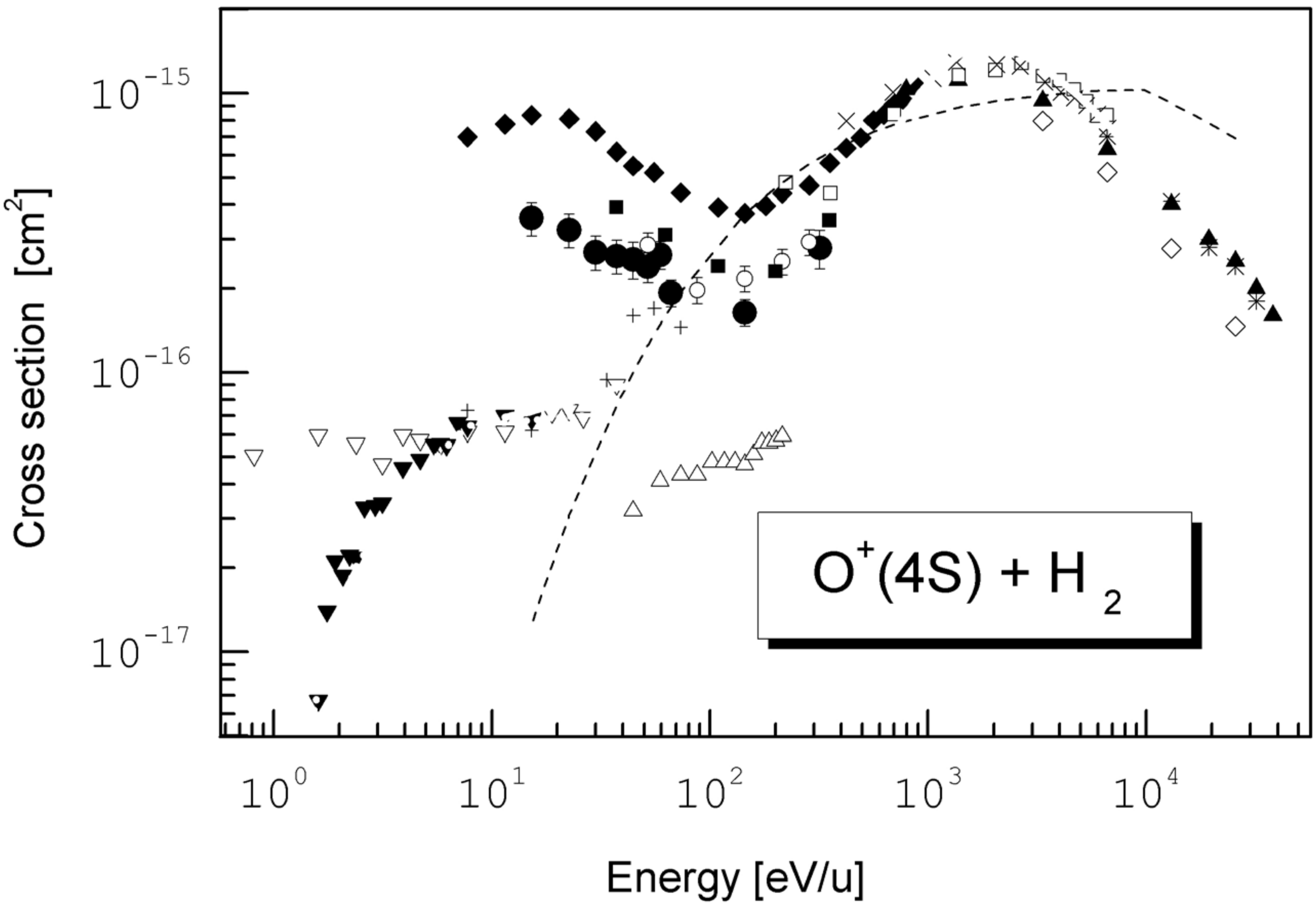
  Important process for astrochemistry and atmospheric science

- 2 sets of the experimental data below ~100 eV

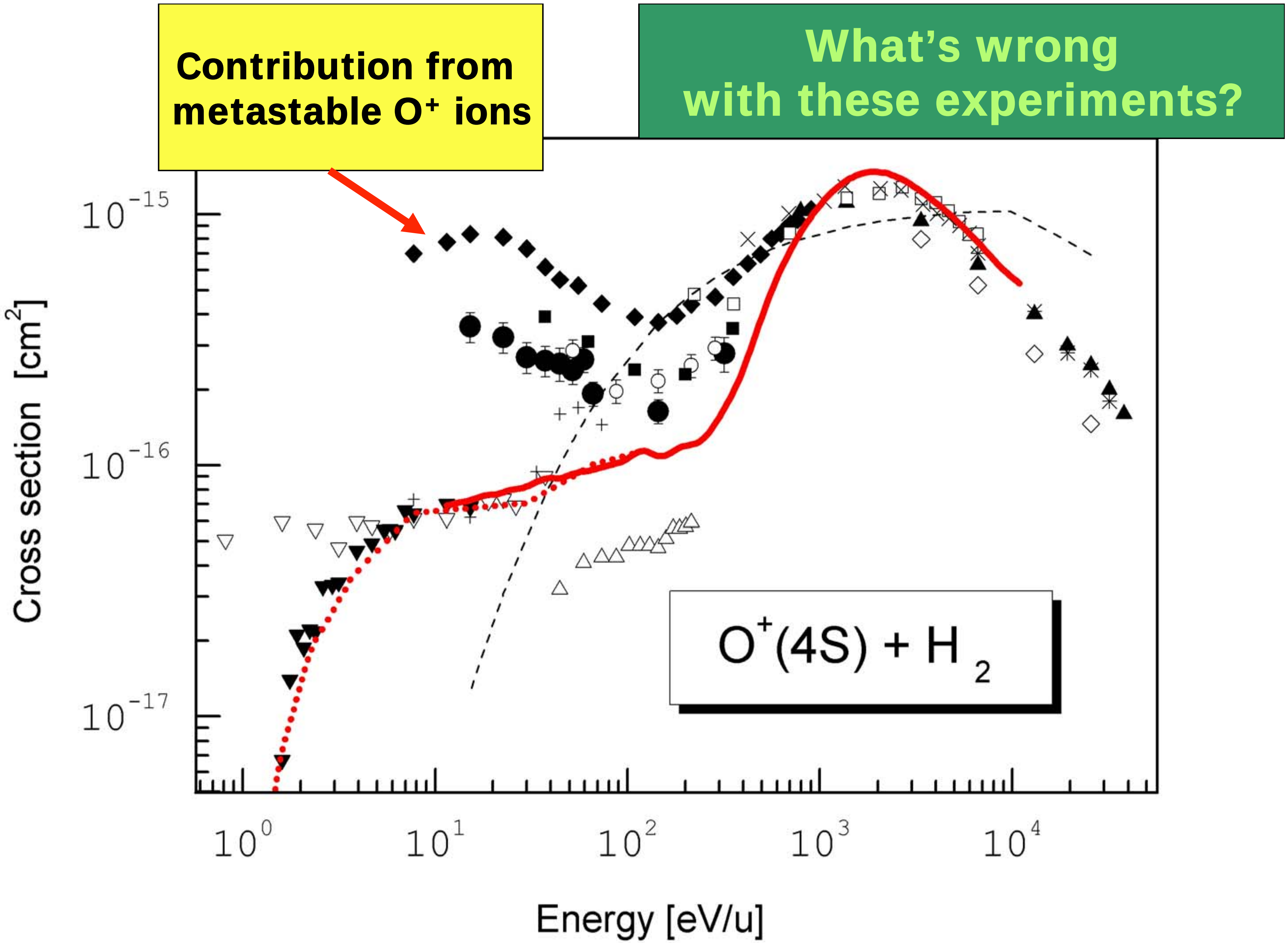
Initial charge transfer reaction for chemistry chains

Cosmic heavy-ions with H2 reaction.

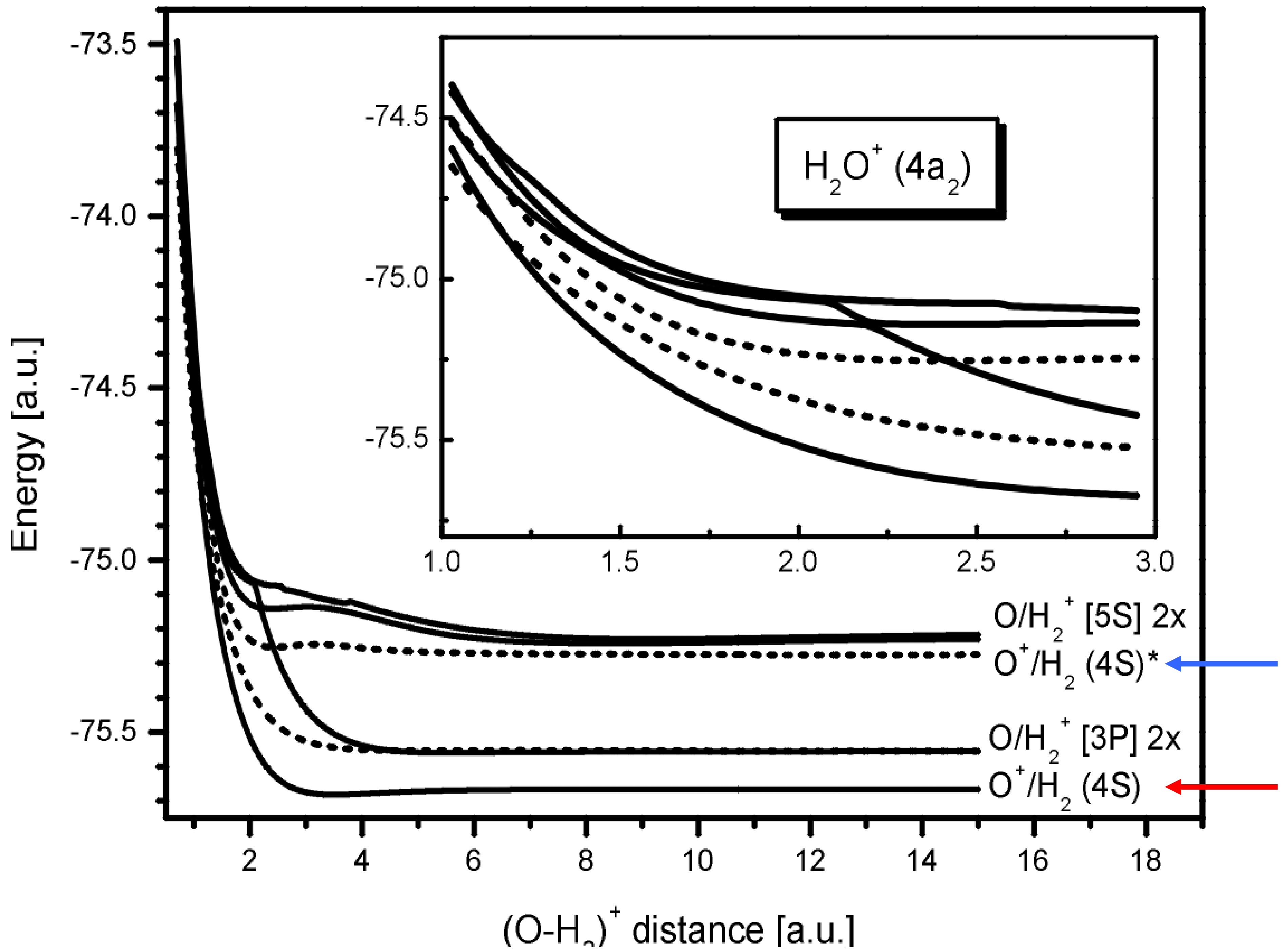
- **$O^+ + H_2 \rightarrow O + H_2^+$**
- **$O^+ + H_2 \rightarrow OH^+ + H$**



Cross section [cm^2]
10^{-15}
10^{-16}
10^{-17}
10^0
10^1
10^2
10^3
10^4
Energy [eV/u]
$O^+(4S) + H_2$



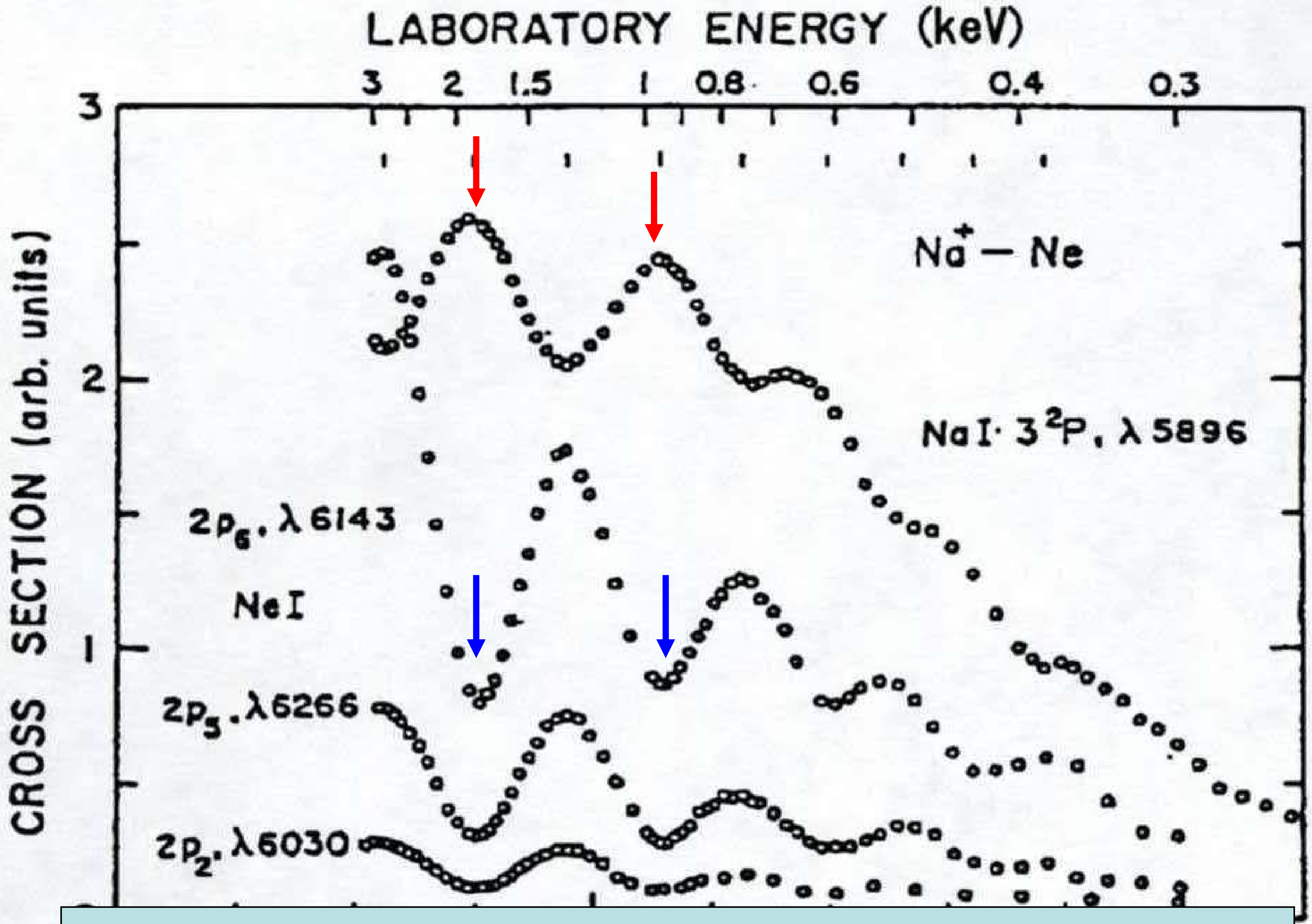
Contribution from metastable O⁺ ions
What's wrong with these experiments?
O+(4S) + H 2
Cross section [cm2]
10-15
10-16
10-17
100
101
102
103
104
Energy [eV/u]



Energy [a.u.]
-73.5
-74.0
-74.5
-75.0
-75.5
2
4
6
8
10
12
14
16
18
(O-H2)+ distance [a.u.]
H2O+ (4a2)
-74.5
-75.0
-75.5
1.0
1.5
2.0
2.5
3.0
O/H2+ [5S] 2x
O+/H2 (4S)*
O/H2+ [3P] 2x
O+/H2 (4S)

Examples of Structures in cross sections

- Interferences
- Resonances
- Structures in partial cross sections
- g-u oscillation
- etc, etc, etc,…..



Rosenthal oscillations:

Na^+ + Ne→Na + Ne^+, Na+ Ne^* processes

Rosenthal oscillations：multi-channel interference

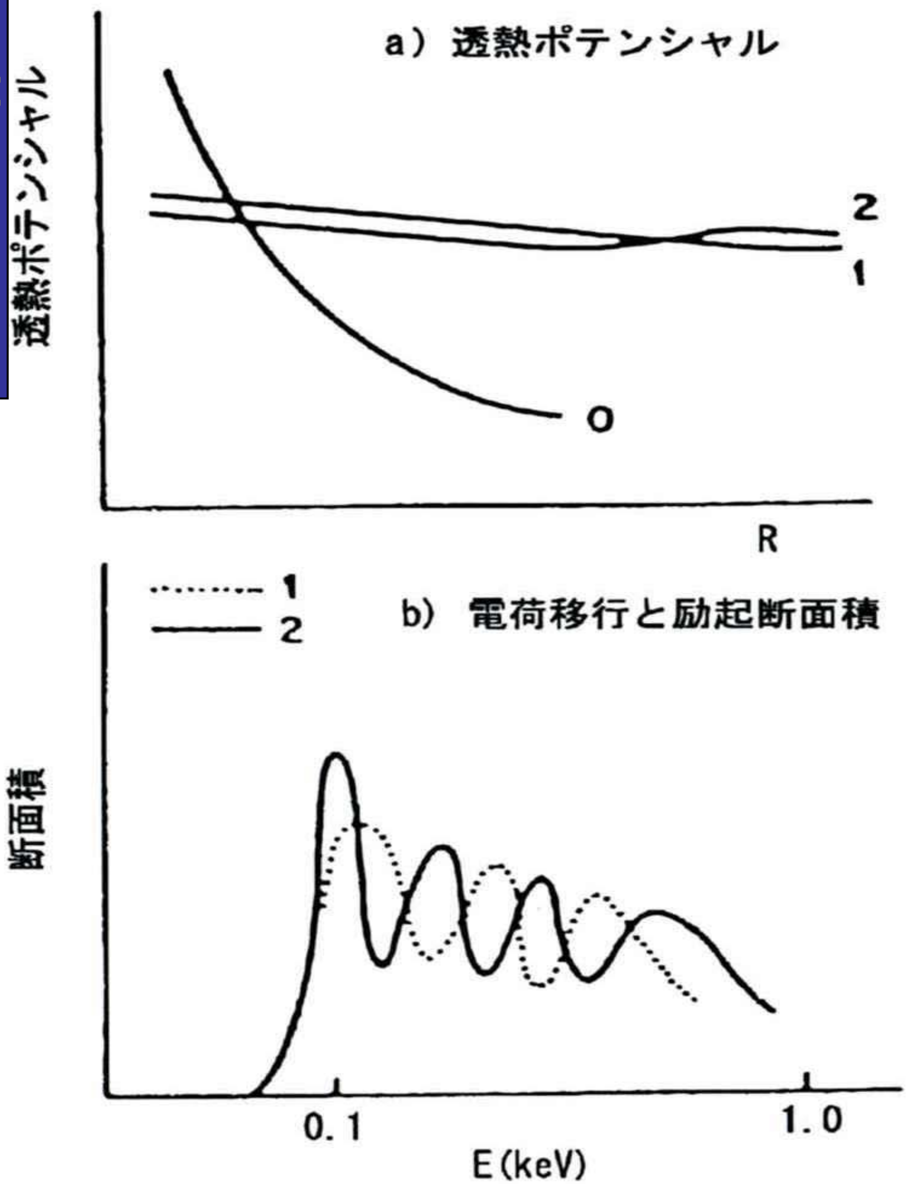


図 2.4.9　Rosenthal 振動のモデル

Structure due to the sum of partial cross sections

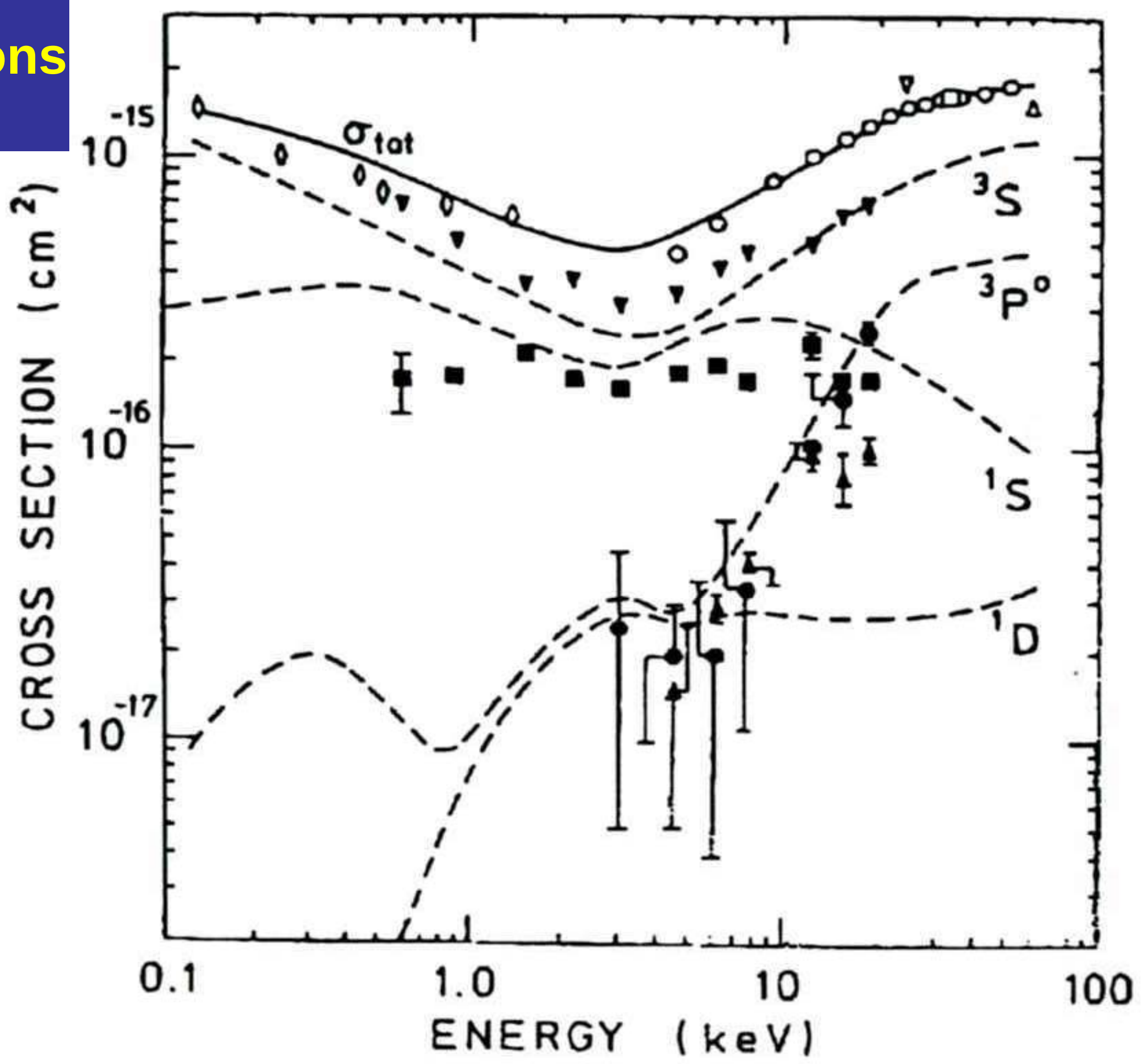
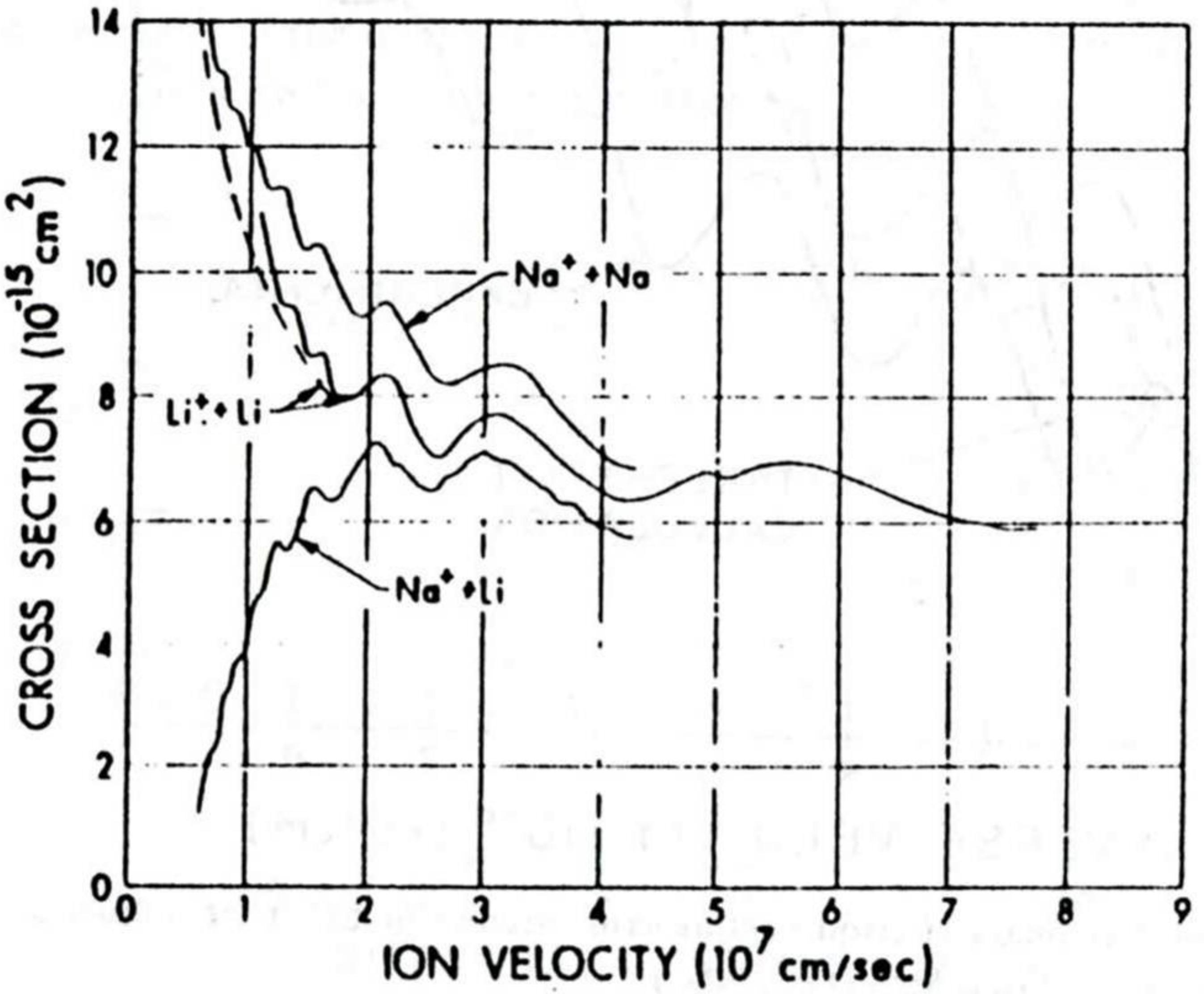


図 **2.4.11** C[5+] + H 衝突の電荷移行過程の部分断面積と全断面積

Smith g-u osillations



PHYSICAL REVIEW A VOLUME 44, NUMBER 3 1 AUGUST 1991

Electron capture in collisions of N^{5+} ions with H atoms from the meV to keV energy regions

N. Shimakura* and M. Kimura
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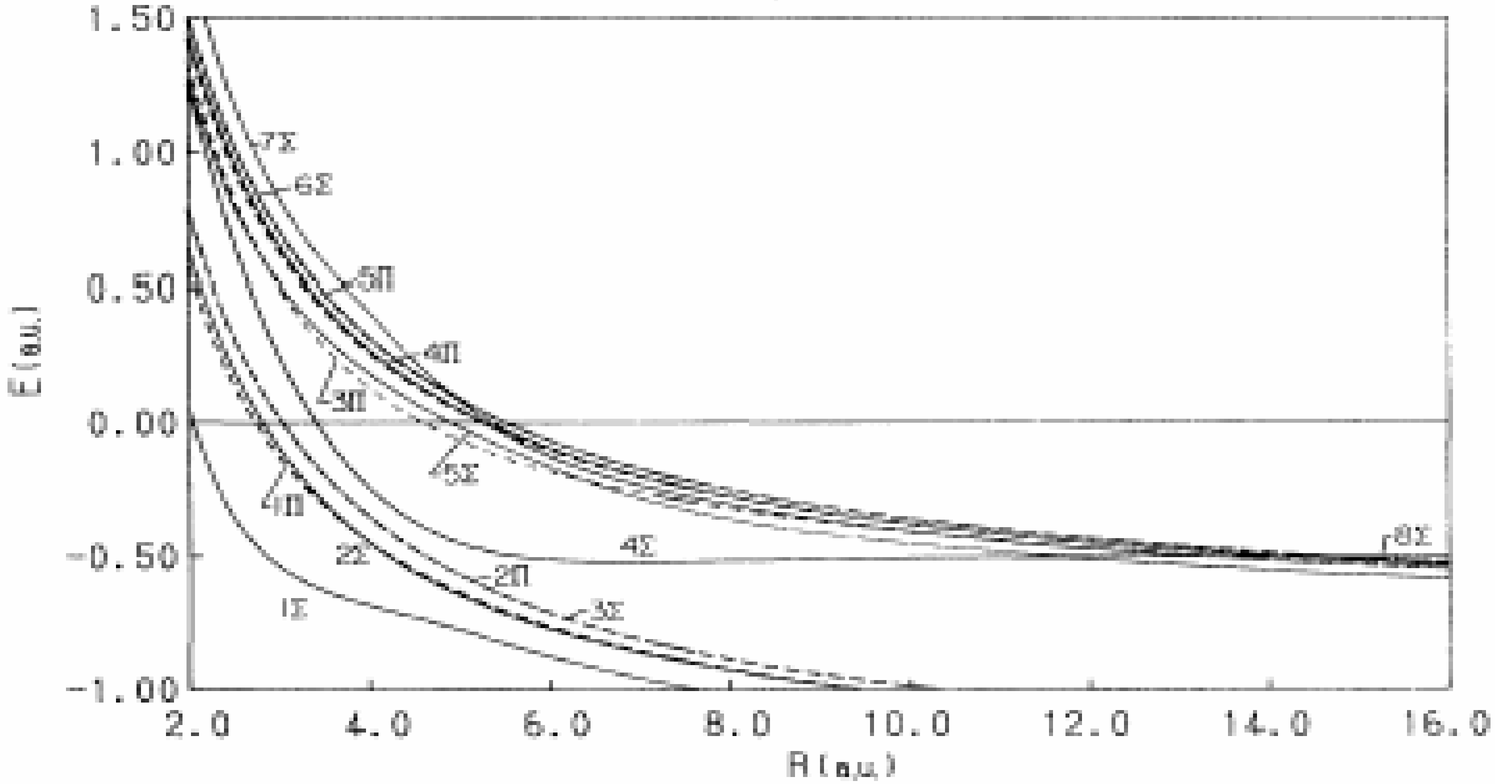
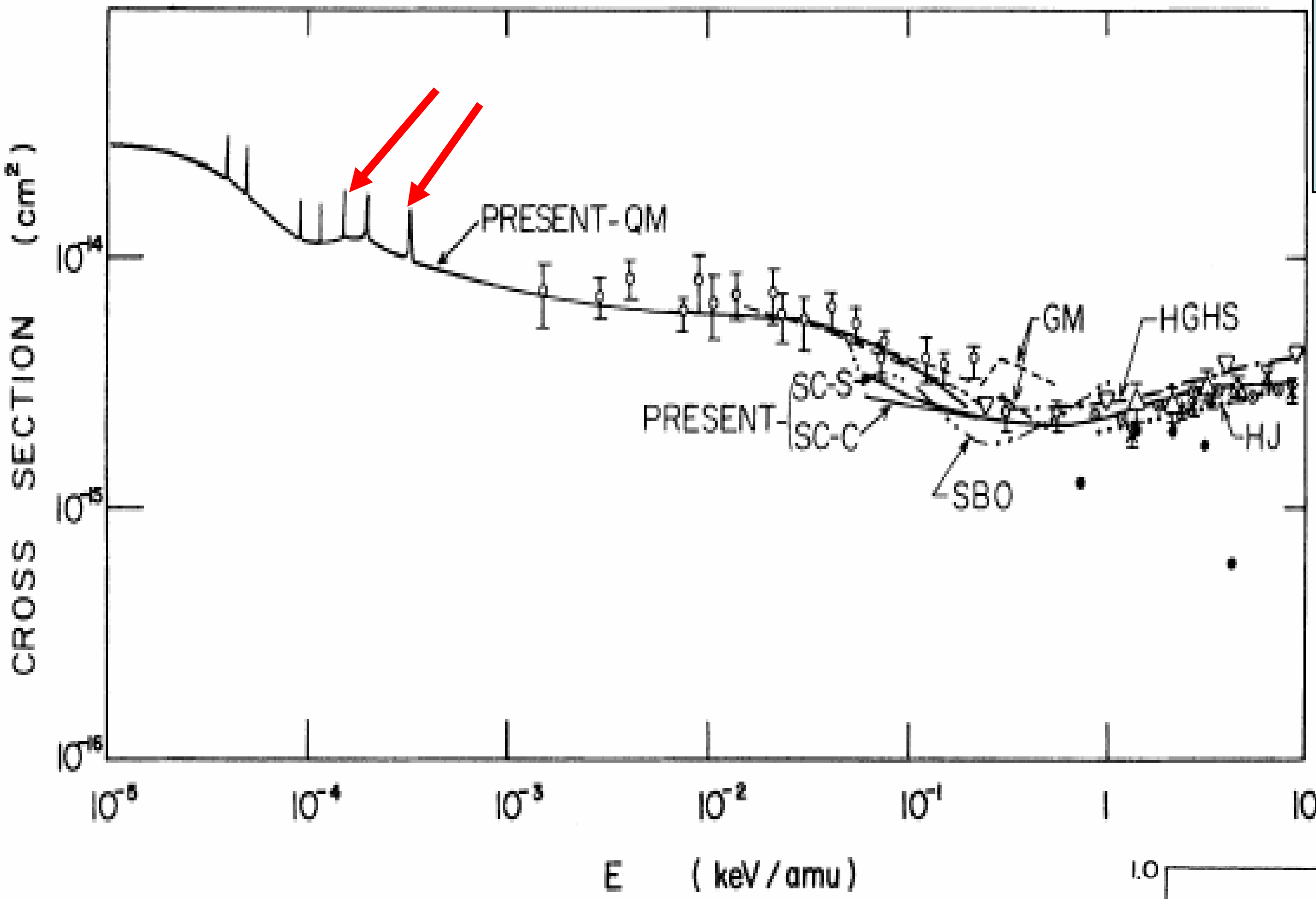
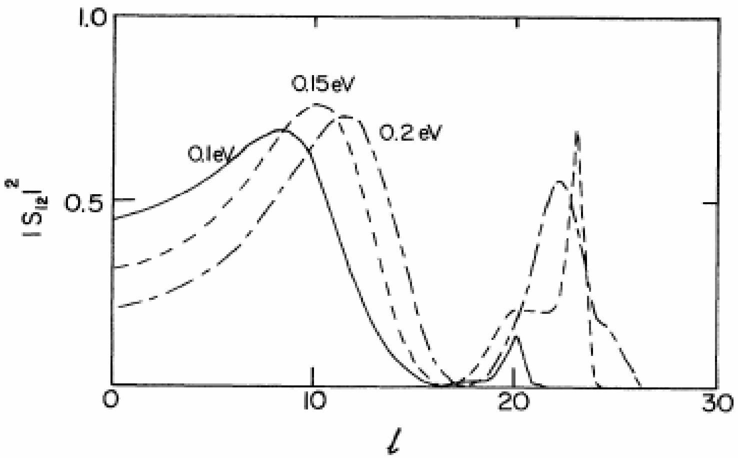
and Department of Physics, Rice University, Houston, Texas 77251





Charge transfer cross sections

Orbiting oscillations (?)



Myths among Atomic Physicists:

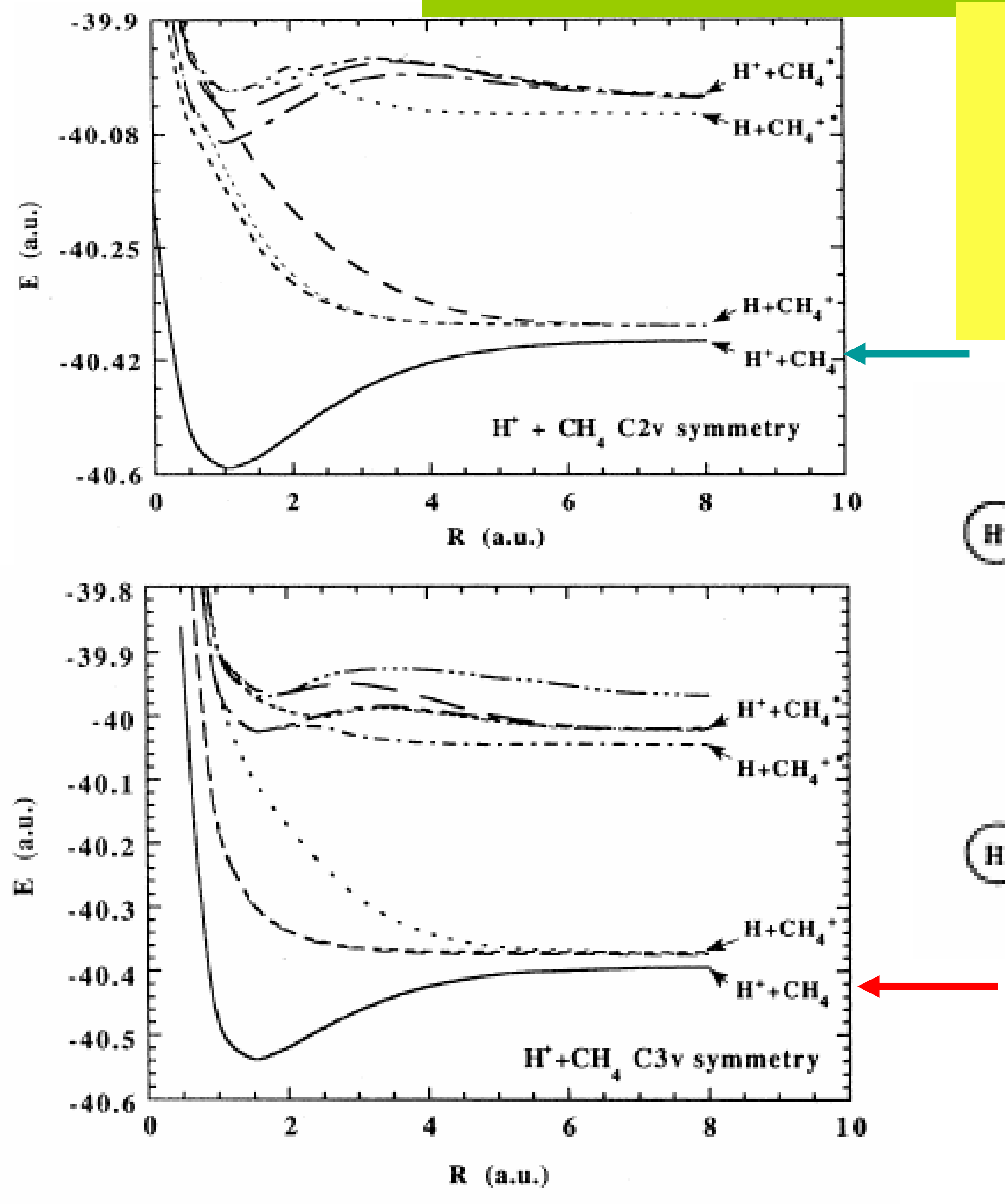
- High eV-keV-energy in collisions
- Collision time 10^{-15} -10^{-17}s

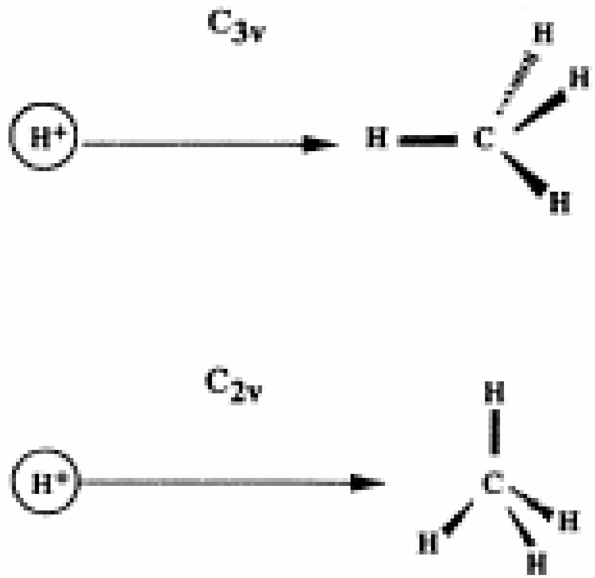
⇨

NO molecular effect, i.e. temperature, and structure effects in high-eV collisions !→NO isotope, isomer..

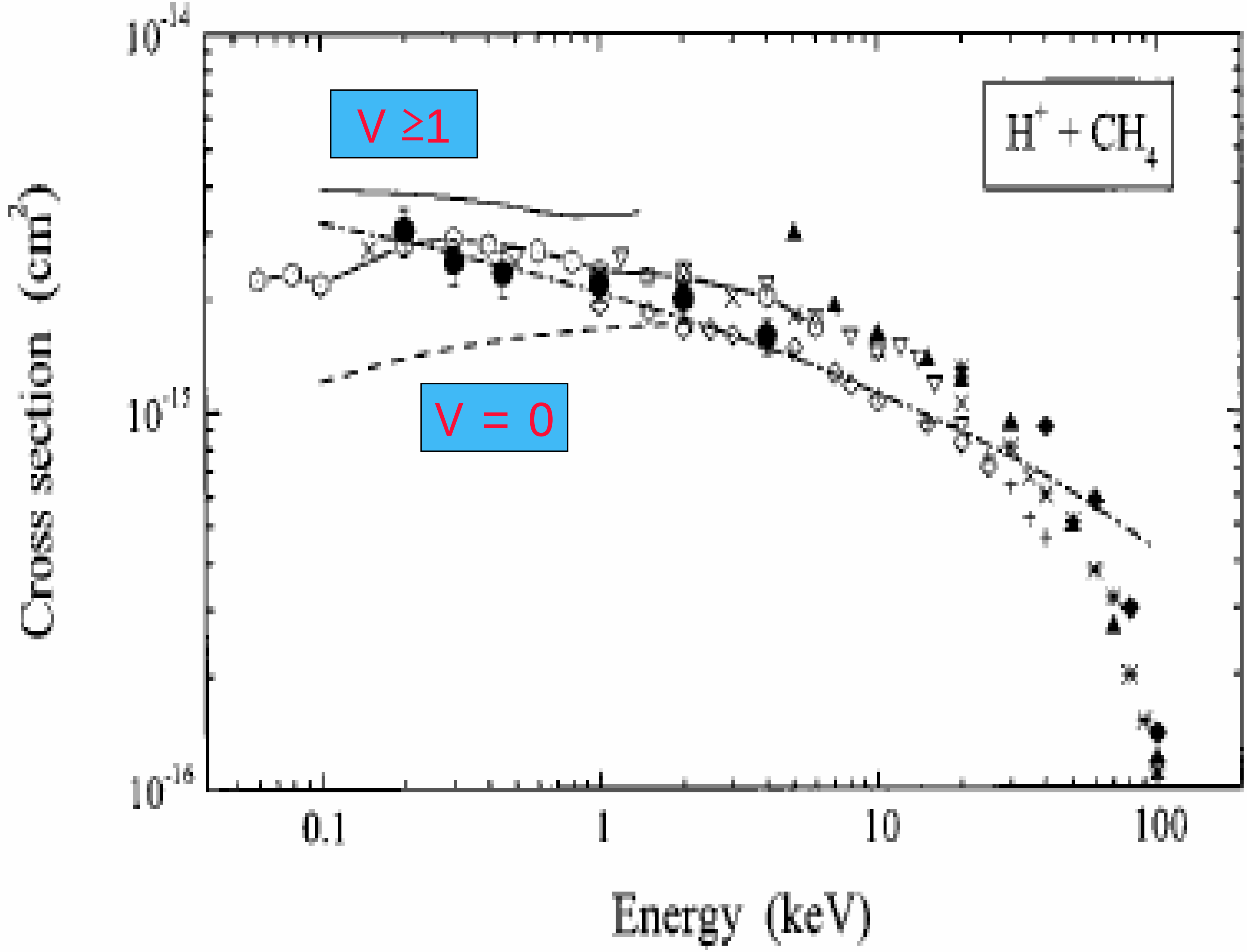
Temperature effect:

H^+ + CH_4 collisions





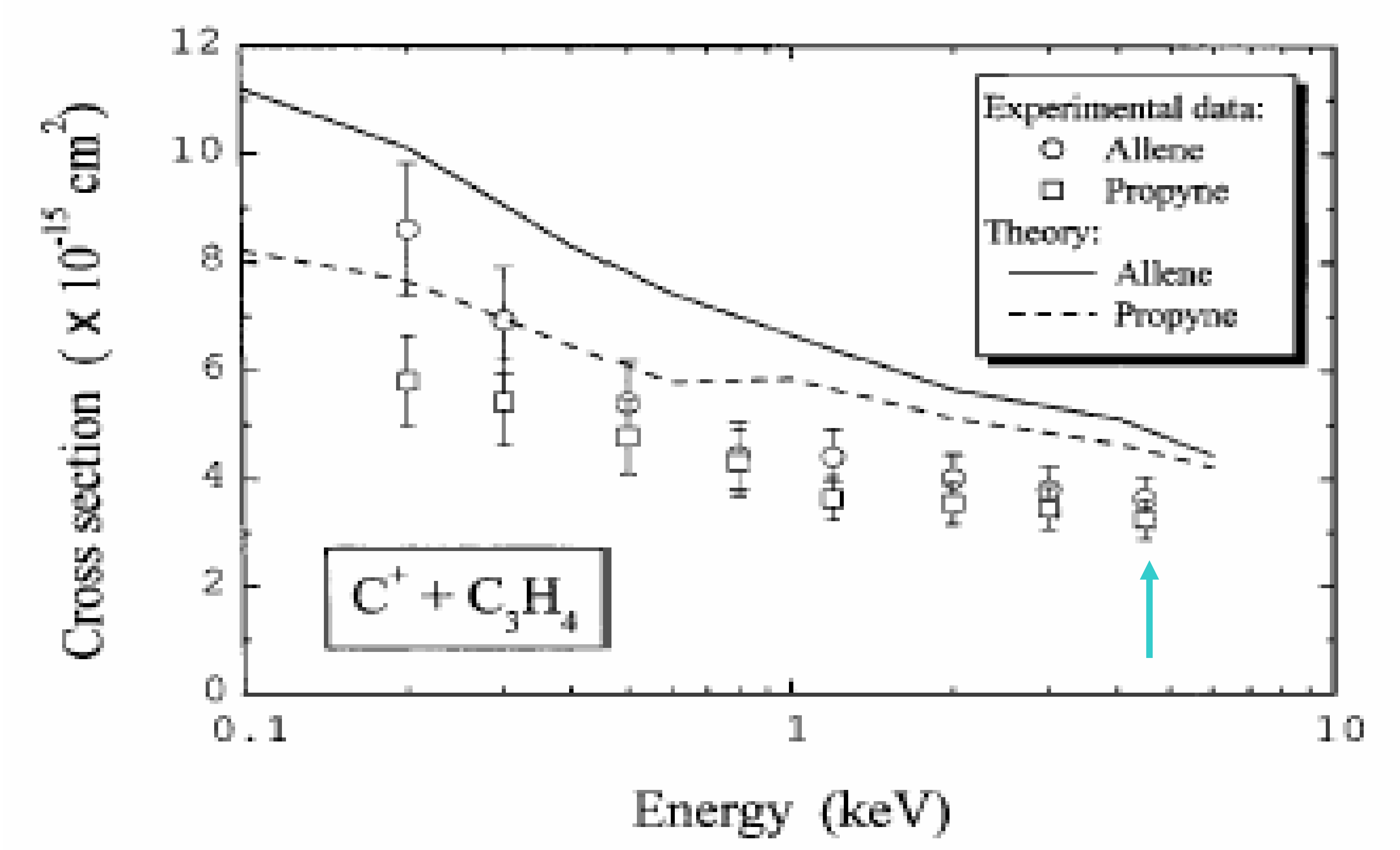
Phys. Rev. A. 62, 062715 (2000).



V ≥1
V = 0
H+ + CH4
Cross section (cm2)
Energy (keV)
10-14
10-15
10-16
0.1
1
10
100

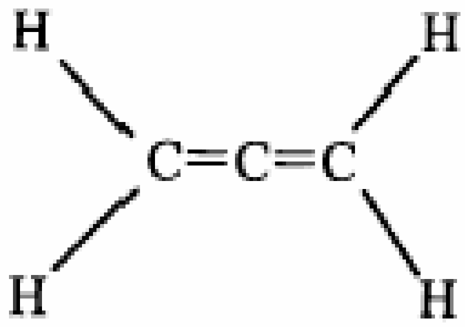
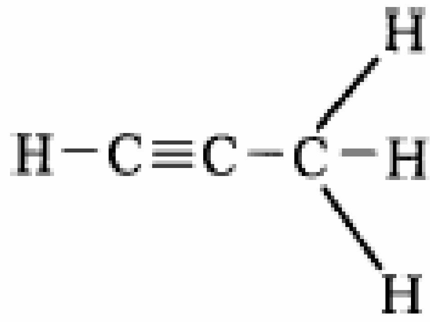
Isomer effect:

CEX in C^+ + C_3H_4 (Allene and Propyne) collisions:

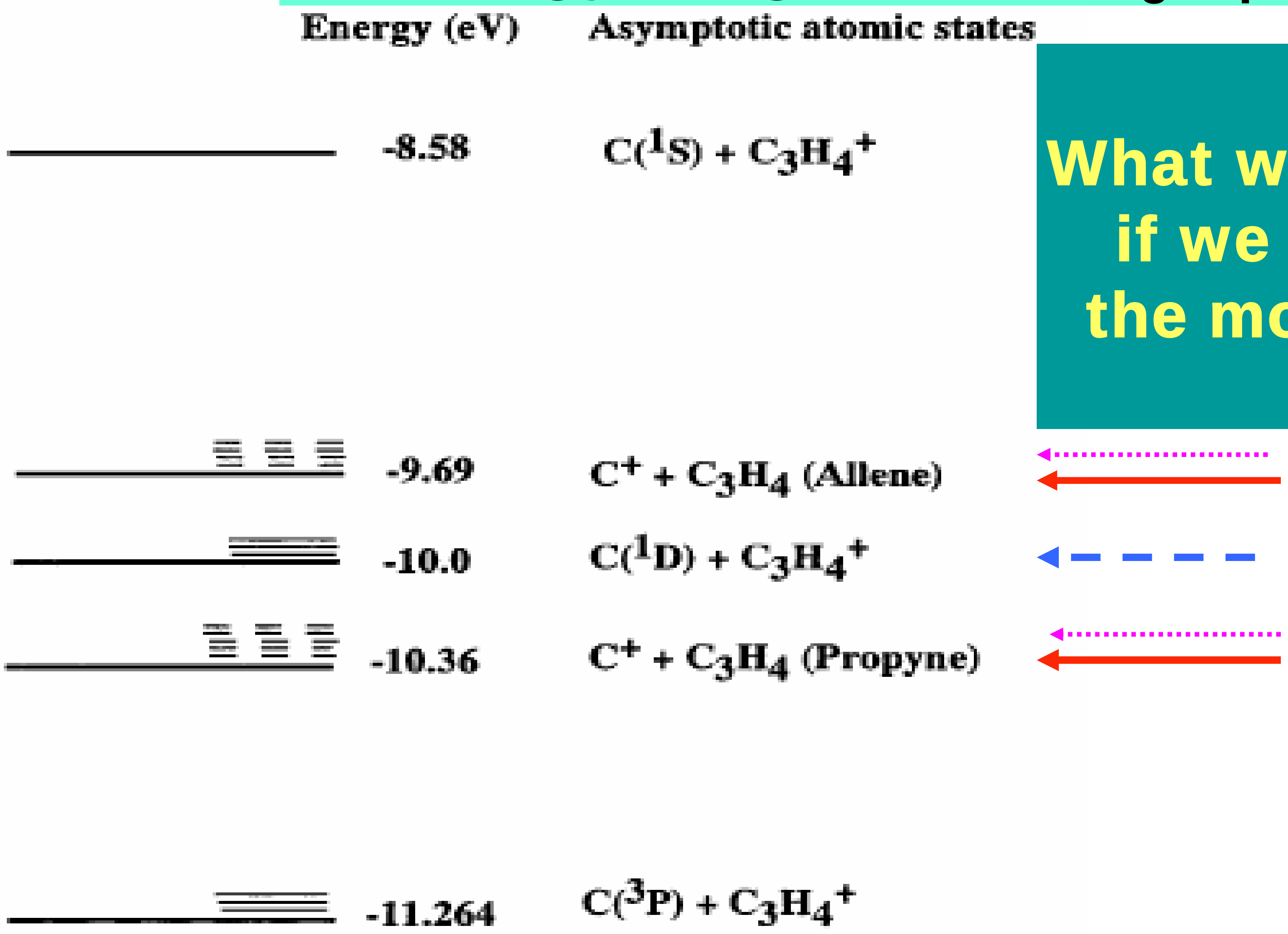


Phys. Rev. Lett. 87, 243201 (2001).

TABLE I. Molecular properties of C_3H_4 (allene and propyne) molecules [8].

Allene		Propyne	
Molecular structure			
			
D_{2d} symmetry		C_{3v} symmetry	
Bond length (Å) and angle			
C-H	1.071	C^3-H	1.112
		C^1-H	1.060
C-C	1.335	C^3-C^2	1.458
		C^2-C^1	1.207
∠HCH	113° ± 1	∠HC^3H	108.4°
Dipole moment (Debye)			
0.2D		0.77D	
Ionization potential (eV)			
9.69 ± 0.01		10.36 ± 0.01	

Energy diagram for C_3H_4



What will happen if we heat up the molecules?

Isotope effect:
$H^+ + H_2$, HD and D_2 collisions

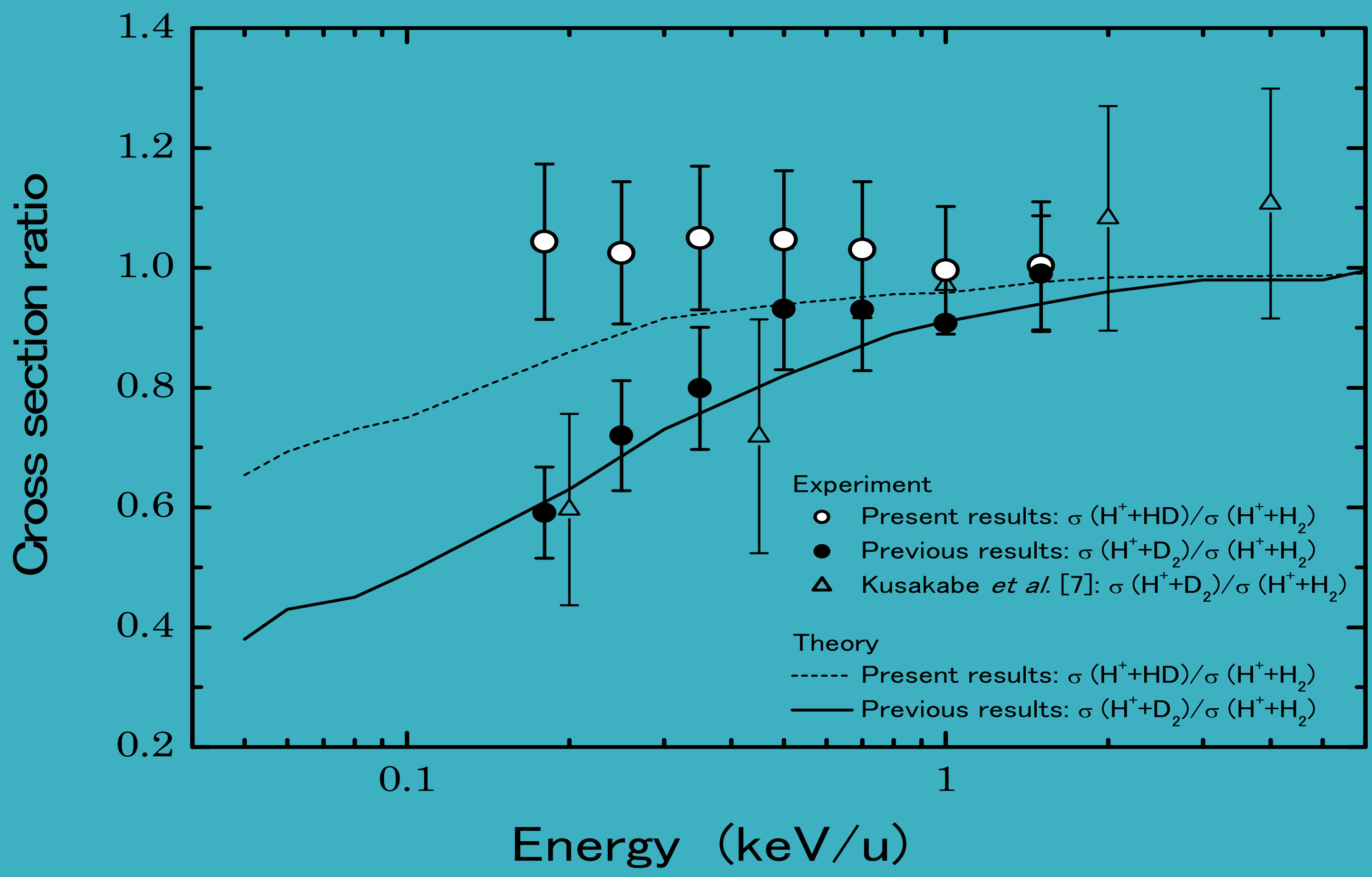


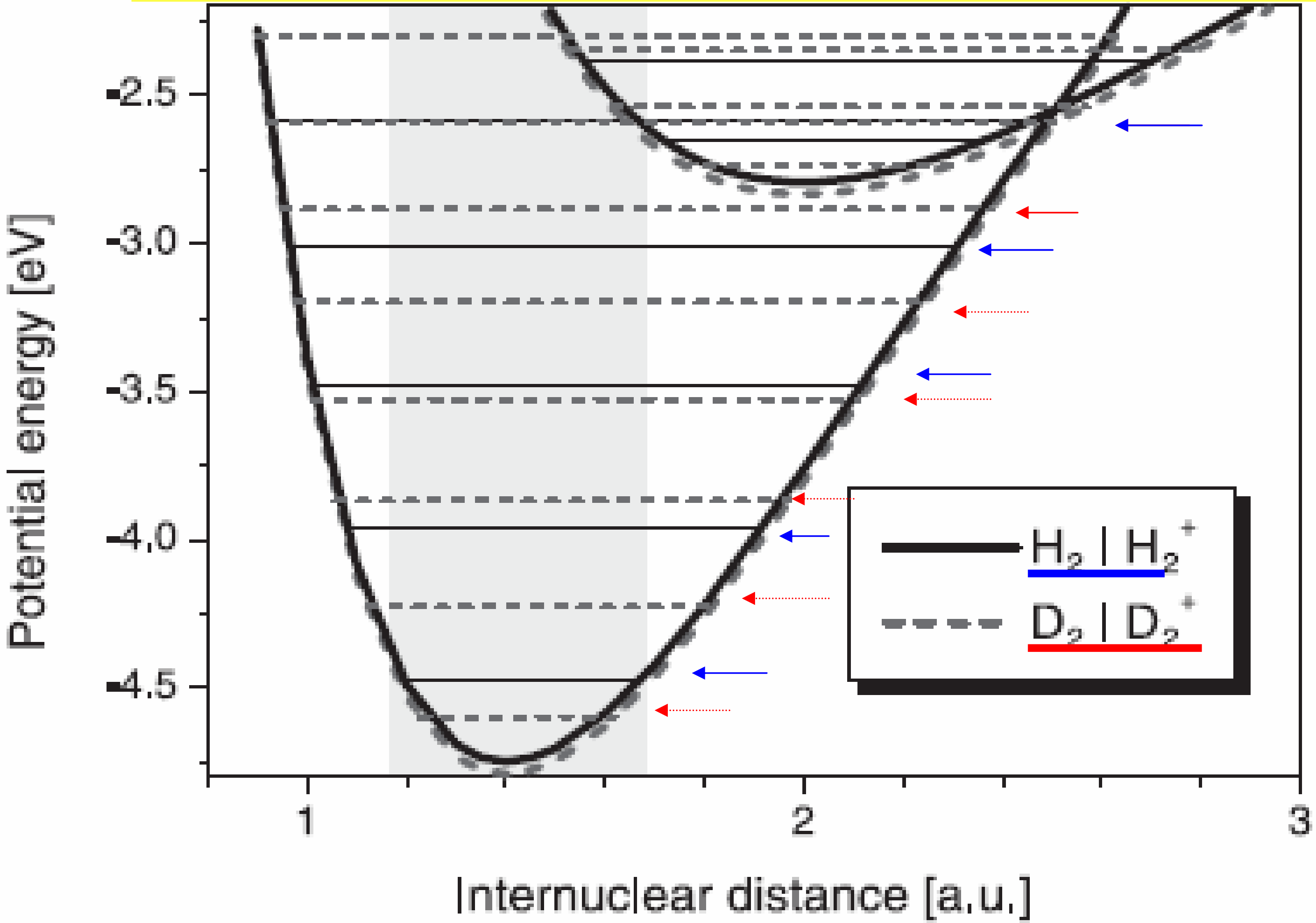
Fig. 5 T. Kusakabe, L.Pichl, M. Kimura et al.

Phys. Rev A.68, Rapid Comm. R050701 (2003).

Molecular constants of H_2, HD, and D_2 molecules.

Molecule	H_2	HD	D_2
Reduced mass (u)	0.504	0.672	1.007
Equilibrium internuclear distance (Å)	0.7414	0.7414	0.7415
Ionization potential (eV)	15.4259	15.445	15.467
Polarizability ($\times 10^{-24}$ cm^3)	0.8023	0.7976	0.7921
Vibrational frequency (cm^{-1})	4401.21	3813.1	3115.5
Vibrational energy (eV)	0.54568	0.47277	0.38628
Dissociation energy (eV)	4.478	4.514	4.556

Adiabatic potential surface for H_2 and D_2



Comment on:

$H^+ + H_2(v=0) \rightarrow H + H_2^+(v')$ dynamics

$H^+ + H_2(v) \rightarrow [H^+ + H_2^*(v')] \rightarrow H + H_2^+(v'')$

Direct excitation through the Franck-Condon factor dominates,

and Intermediate vibrational excitation channels are not significant

VOLUME 91, NUMBER 5 PHYSICAL REVIEW LETTERS week ending 1 AUGUST 2003

Charge Driven Fragmentation of Nucleobases

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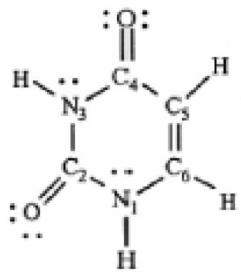
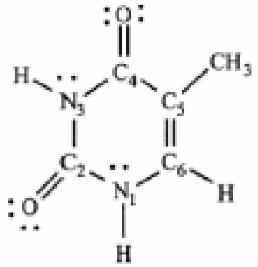
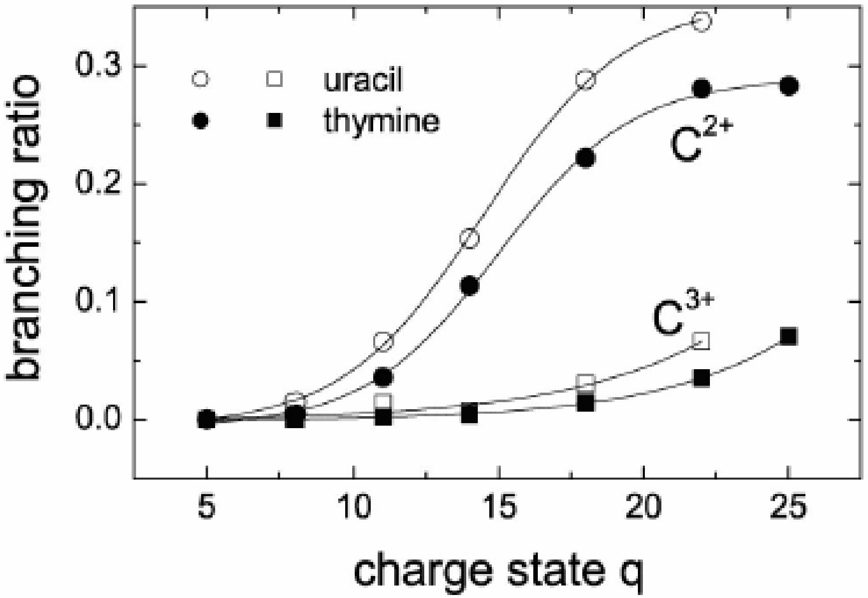
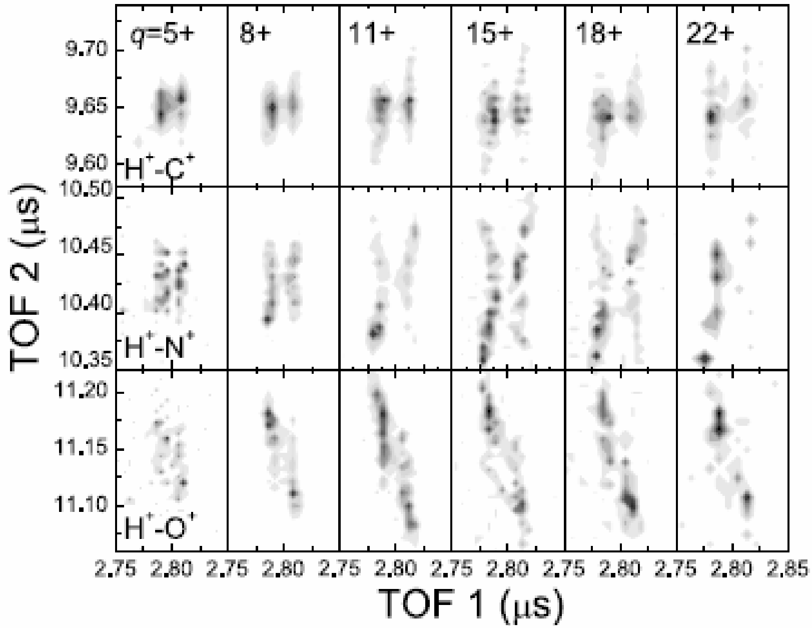
uracil

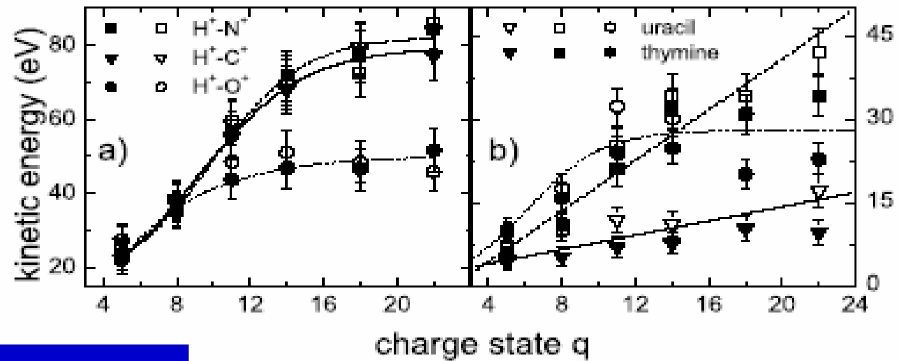


thymine









Fragmentation of DNA bases by ions

Beyond the Bragg Peak: Hyperthermal Heavy Ion Damage to DNA Components

Zongwu Deng, Ilko Bald,* Eugen Illenberger,* and Michael A. Huels†

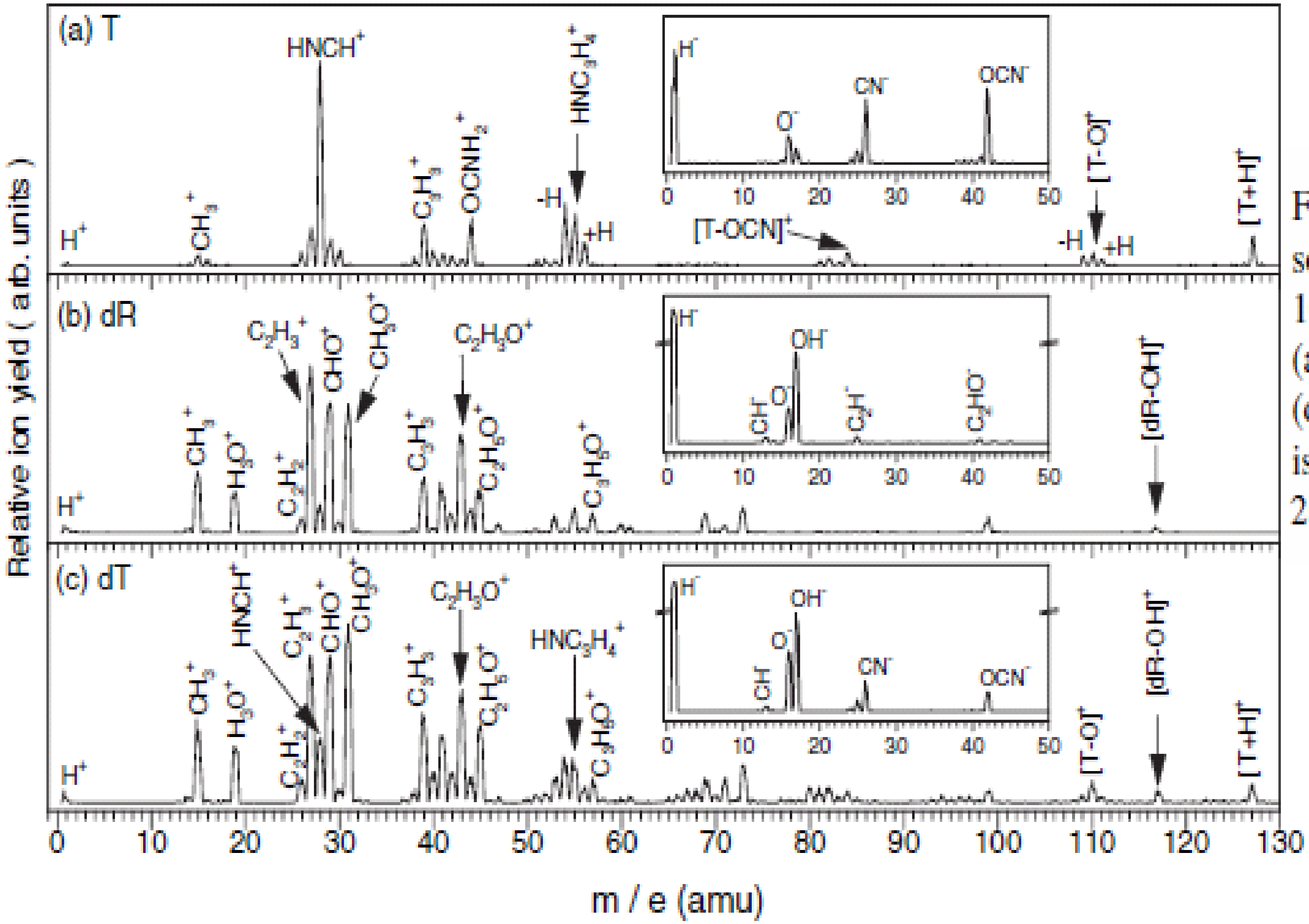


FIG. 1. Cation and anion (insets) desorption mass spectra produced by 100 eV Ar^+ impact on films of (a) thymine (T), (b) 2-deoxy-D-ribose (dR), and (c) thymidine (dT); each film is about 4 nominal monolayers (4 ML ≈ 200 ng/cm^2) on a Pt substrate.

Outstanding problems

- There are a lot for us to do investigating physics of ION, ELECTRON, PHOTON COLLISIONS!!
- There are a lot for us to do to provide complete, and accurate cross section data for applications.
- Particularly ion-molecules studies for low-energies.

How to encourage experimentalists to study these collisions for various species in wide range of energies, etc, etc ?

How to encourage theorists to tackle Atomic collision problems and calculate accurate cross sections ?

Acknowledgement

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H.-P. Liebermann	Max-Planck Institut-Heidelberg
Alex Dalgarno	Harvard University
Cliff Surko	UC-San Diego

- **$$$**

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National Institute for Radiological Sciences