酸素分子と電子の衝突に関する最近の研究

市川行和

J. Phys. Chem. Ref. Data 38, 1 (2009)

Cross Sections for Electron Collisions with Oxygen Molecules

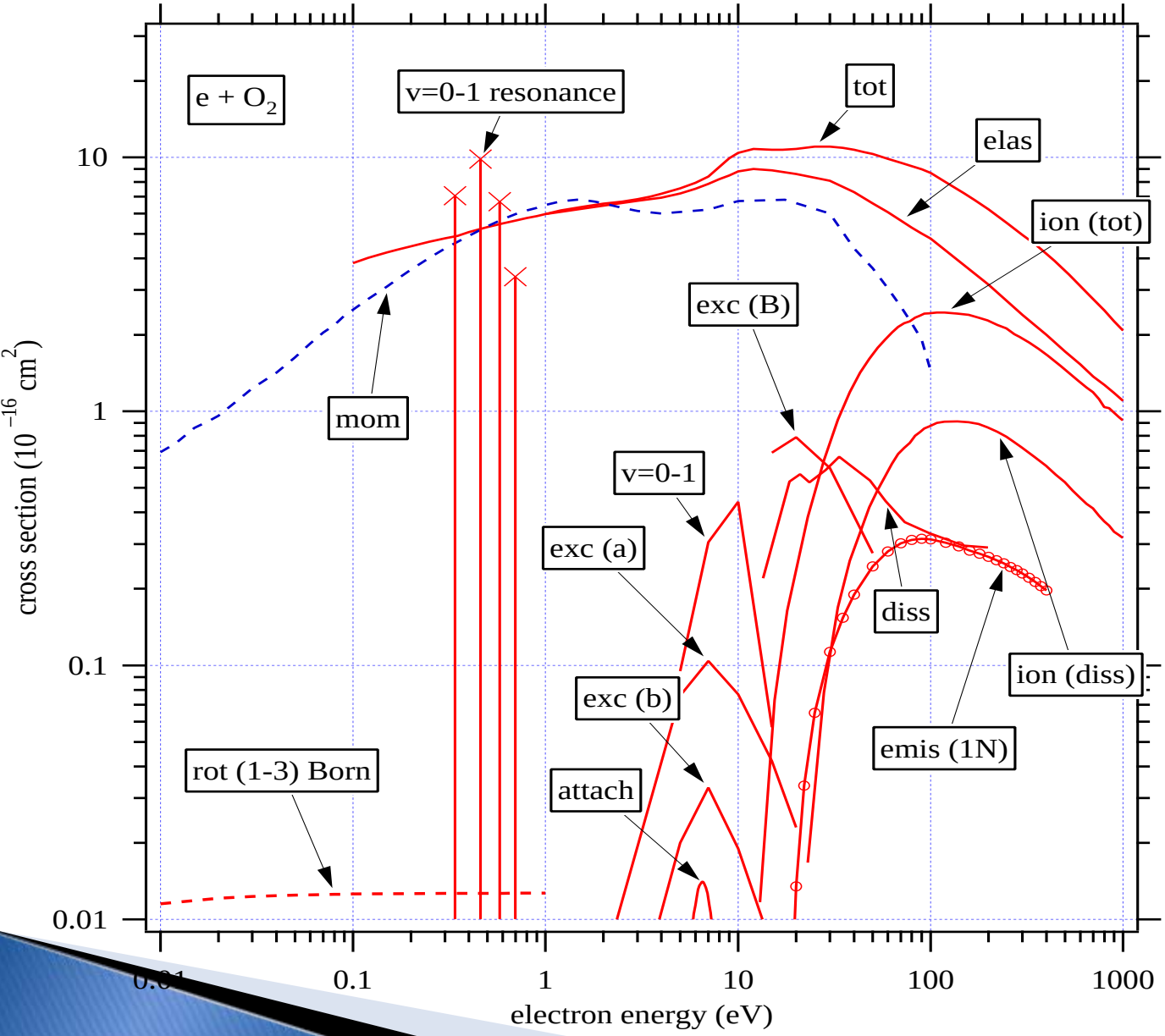
Yukikazu Itikawa[a)]

Institute of Space and Astronautical Science, Sagamihara 229-8510, Japan

(Received 8 July 2008; accepted 23 October 2008; published online 12 December 2008)

Cross section data are collected and reviewed for electron collisions with oxygen molecules. Included are the cross sections for total and elastic scatterings, momentum transfer, excitations of rotational, vibrational, and electronic states, dissociation, ionization, electron attachment, and emission of radiations. For each process, the recommended values of the cross sections are presented, when possible. The literature has been surveyed through the end of 2007.
[DOI: 10.1063/1.3025886]

O_2 Itikawa, JPCRD 38, 1 (2009)



今後の課題(2008)

電子状態励起

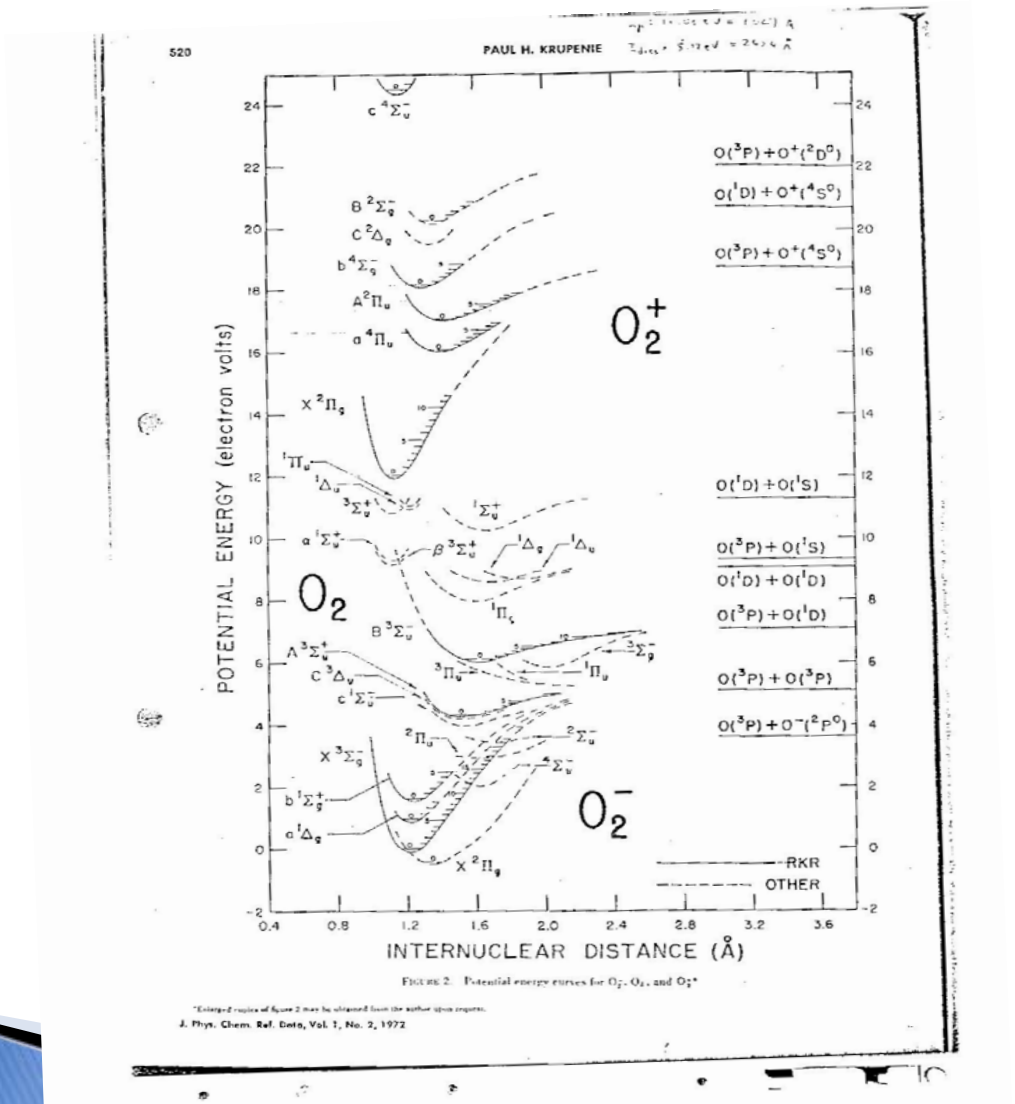
　　データの不一致

回転励起

　　実験なし

解離の詳細

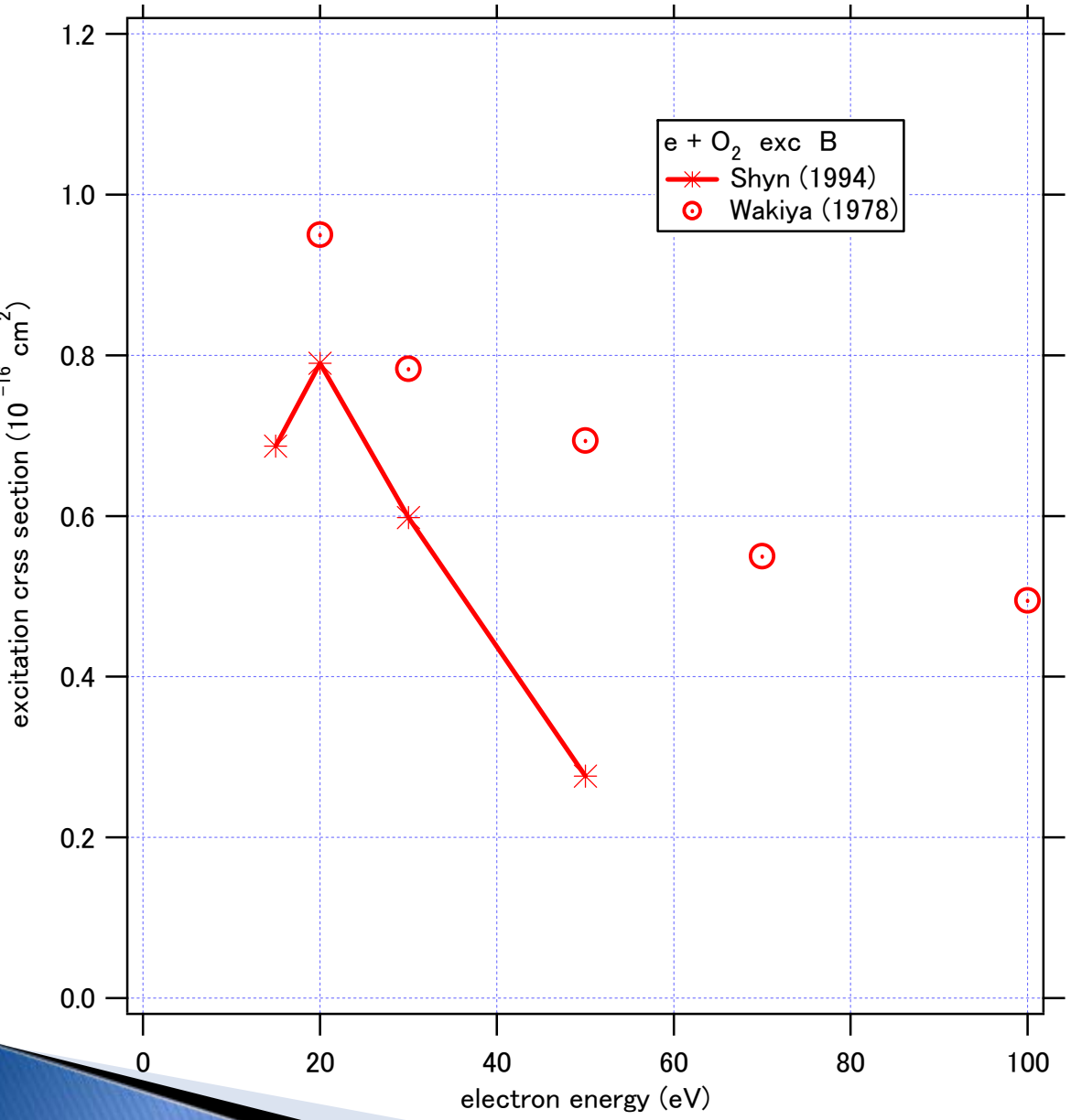
酸素分子の電子状態


520
PAUL H. KRUPENIE
POTENTIAL ENERGY (electron volts)
INTERNUCLEAR DISTANCE (Å)
O_2^+
O_2
O_2^-
$c\,^4\Sigma_u^-$
$B\,^2\Sigma_g^-$
$C\,^2\Delta_g$
$b\,^4\Sigma_g^-$
$A\,^2\Pi_u$
$a\,^4\Pi_u$
$X\,^2\Pi_g$
$^1\Pi_u$
$^1\Delta_u$
$^3\Sigma_u^+$
$^1\Sigma_u^+$
$a\,^1\Sigma_u^+$
$\beta\,^3\Sigma_u^+$
$^1\Delta_g$
$^1\Pi_g$
$B\,^3\Sigma_u^-$
$A\,^3\Sigma_u^+$
$C\,^3\Delta_u$
$c\,^1\Sigma_u^-$
$^3\Pi_u$
$^3\Sigma_g^-$
$^1\Pi_u$
$^2\Pi_u$
$^2\Sigma_u^-$
$X\,^3\Sigma_g^-$
$b\,^1\Sigma_g^+$
$a\,^1\Delta_g$
$X\,^2\Pi_g$
$^2\Sigma_u^-$
$O(^3P)+O^+(^2D^o)$
$O(^1D)+O^+(^4S^o)$
$O(^3P)+O^+(^4S^o)$
$O(^1D)+O(^1S)$
$O(^3P)+O(^1S)$
$O(^1D)+O(^1D)$
$O(^3P)+O(^1D)$
$O(^3P)+O(^3P)$
$O(^3P)+O^-(^2P^o)$
RKR
OTHER
FIGURE 2. Potential energy curves for O_2^-, O_2, and O_2^+
J. Phys. Chem. Ref. Data, Vol. 1, No. 2, 1972

$O_2\,(X) \rightarrow \; O_2\,(B\,^3\Sigma_u^-)$

実験

- Wakiya J.Phys.B 11, 3913 (1978)
- Shyn et al. Phys.Rev A 50, 4794 (1994)


e + O2 exc B
Shyn (1994)
Wakiya (1978)
excitation crss section (10^-16 cm^2)
electron energy (eV)
0.0
0.2
0.4
0.6
0.8
1.0
1.2
0
20
40
60
80
100

Before 2008

JPCRD (2009)

recommends
Shyn et al. (1994)

but more experiments should be done

In 2010
a new measurement by
Tanaka's group at Sophia Univ.

J. Chem. Phys. 134, 064311 (2011)

THE JOURNAL OF CHEMICAL PHYSICS **134**, 064311 (2011)

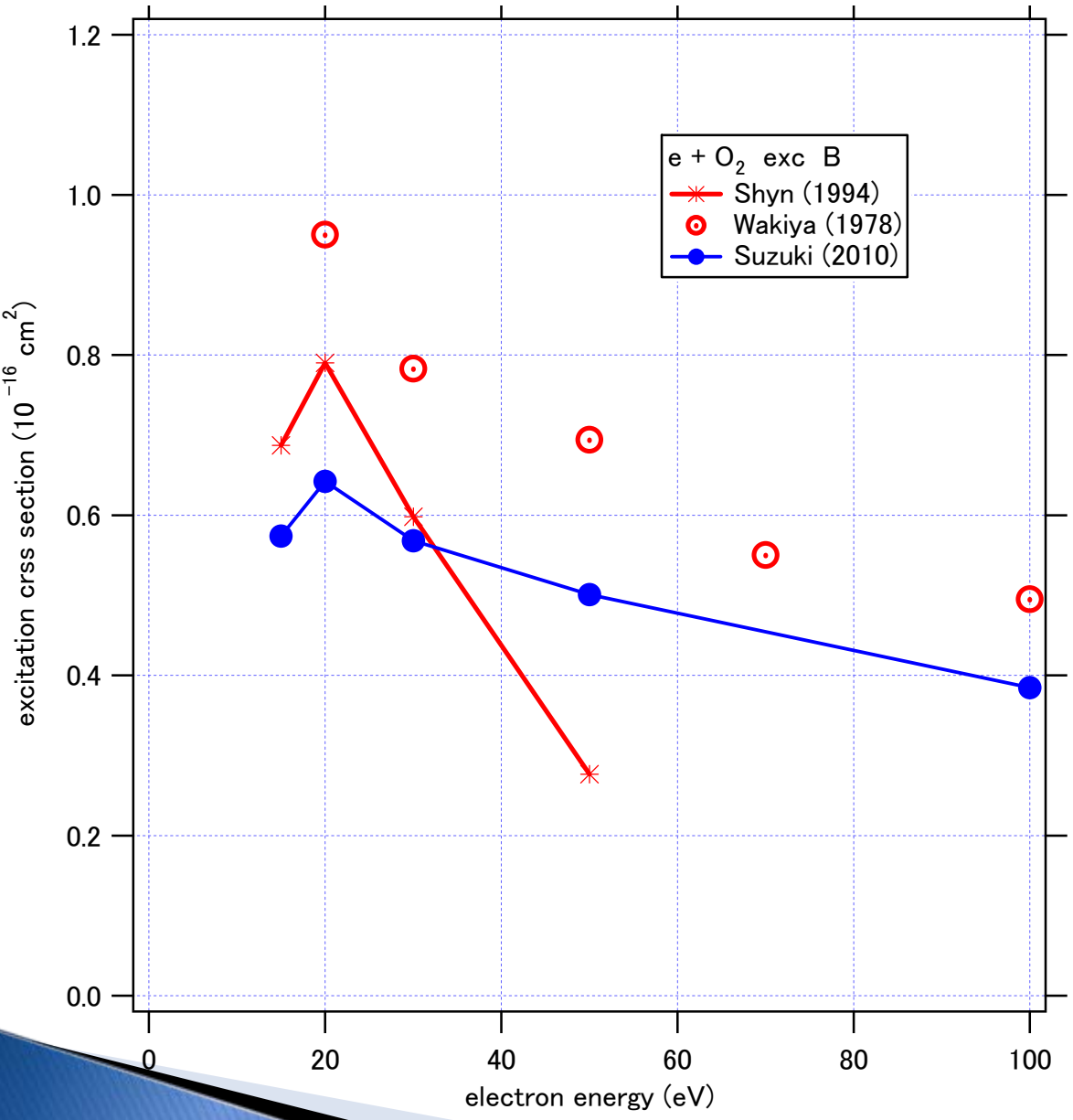
Electron excitation of the Schumann–Runge continuum, longest band, and second band electronic states in O_2

Daisuke Suzuki,[1] Hidetoshi Kato,[1] Mizuha Ohkawa,[1] Kazutoshi Anzai,[1] Hiroshi Tanaka,[1] Paulo Limão-Vieira,[2] Laurence Campbell,[3] and Michael J. Brunger[3,a)]

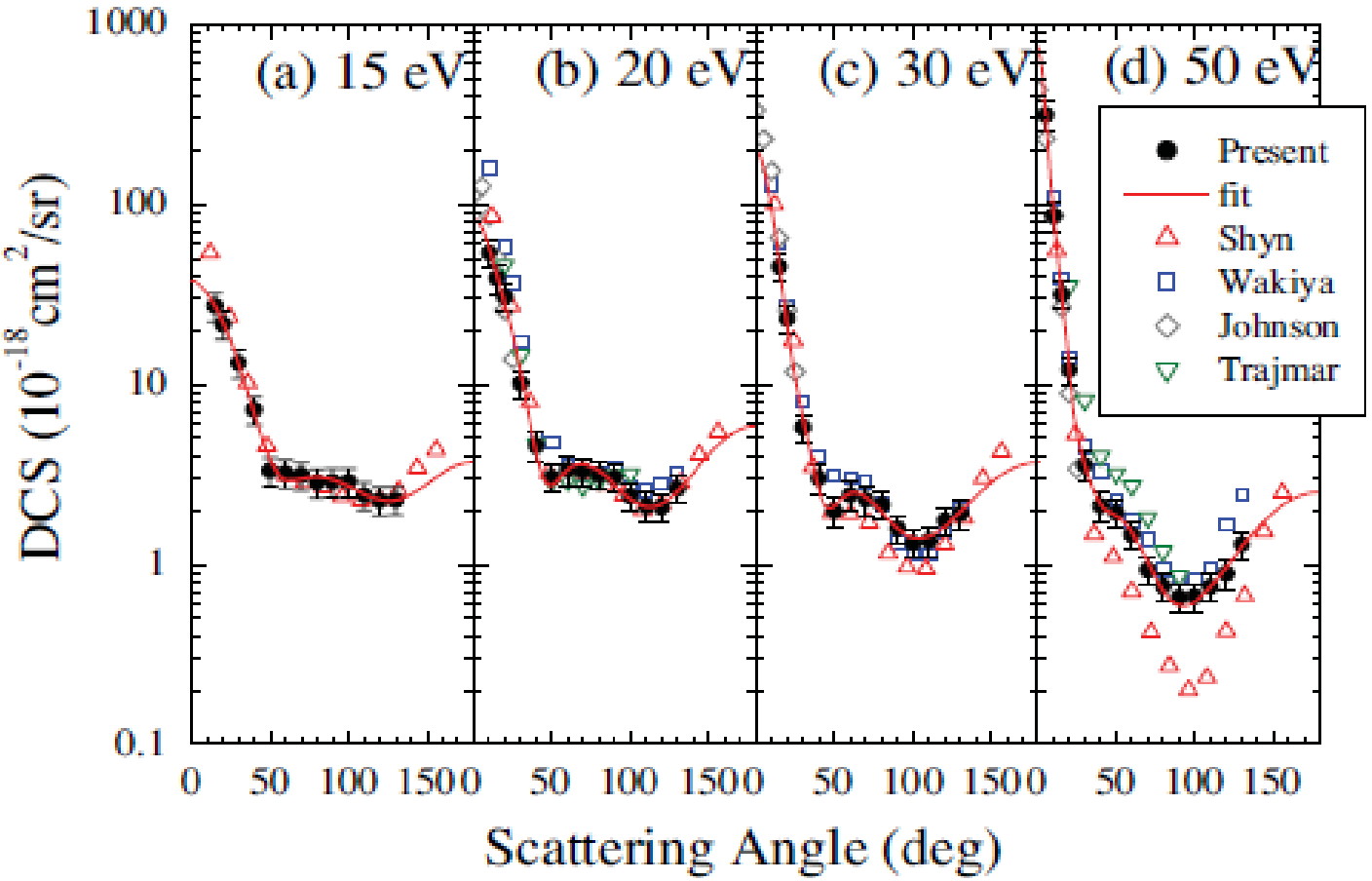
[1]*Department of Physics, Sophia University, Chiyoda-ku, Tokyo 102-8554, Japan*

[2]*Laboratório de Colisões Atómicas e Moleculares, Departamento de Física, CEFITEC, Universidade Nova de Lisboa, P-2829-516 Caparica, Portugal*

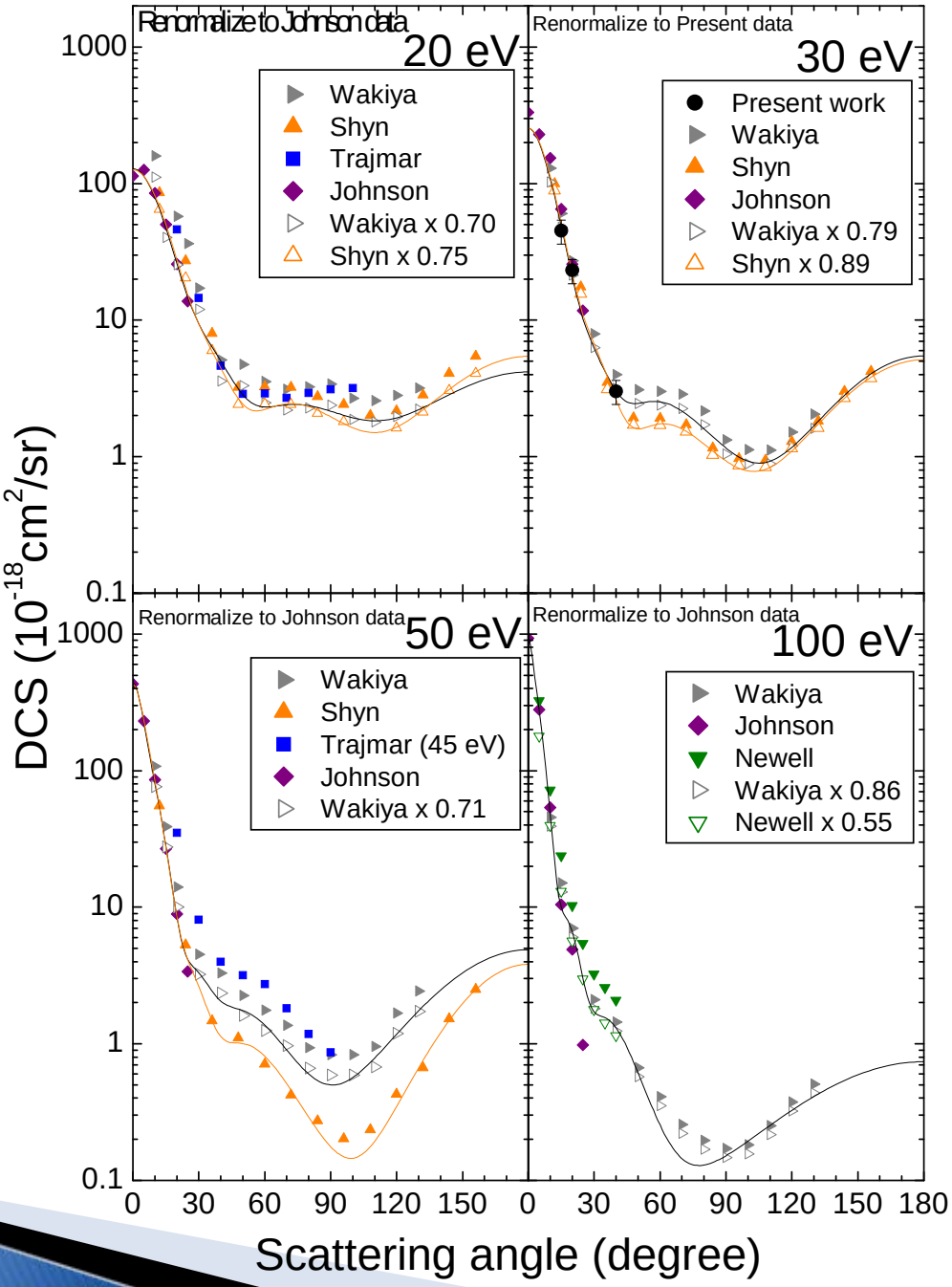
[3]*ARC Centre for Antimatter-Matter Studies, School of Chemical and Physical Sciences, Flinders University, GPO Box 2100, Adelaide, South Australia 5001, Australia*



Which is the best ?


(a) 15 eV
(b) 20 eV
(c) 30 eV
(d) 50 eV
Present
fit
Shyn
Wakiya
Johnson
Trajmar
DCS (10^{-18} cm^2/sr)
Scattering Angle (deg)
1000
100
10
1
0.1
0
50
100
150

Schumann-Runge



評価の手法（その一）

スケール則の活用

The Born method

For the dipole-allowed transition
like O_2 (X) → O_2 (B)

the Born approximation gives
a good result at a high energy (> 100 eV)

Born 近似の低エネルギー部分を修正して、全エネルギー範囲で使う試み

Scaling by Yong-Ki Kim

To extend the Born c.s. toward lower energies, Kim proposed a scaling method

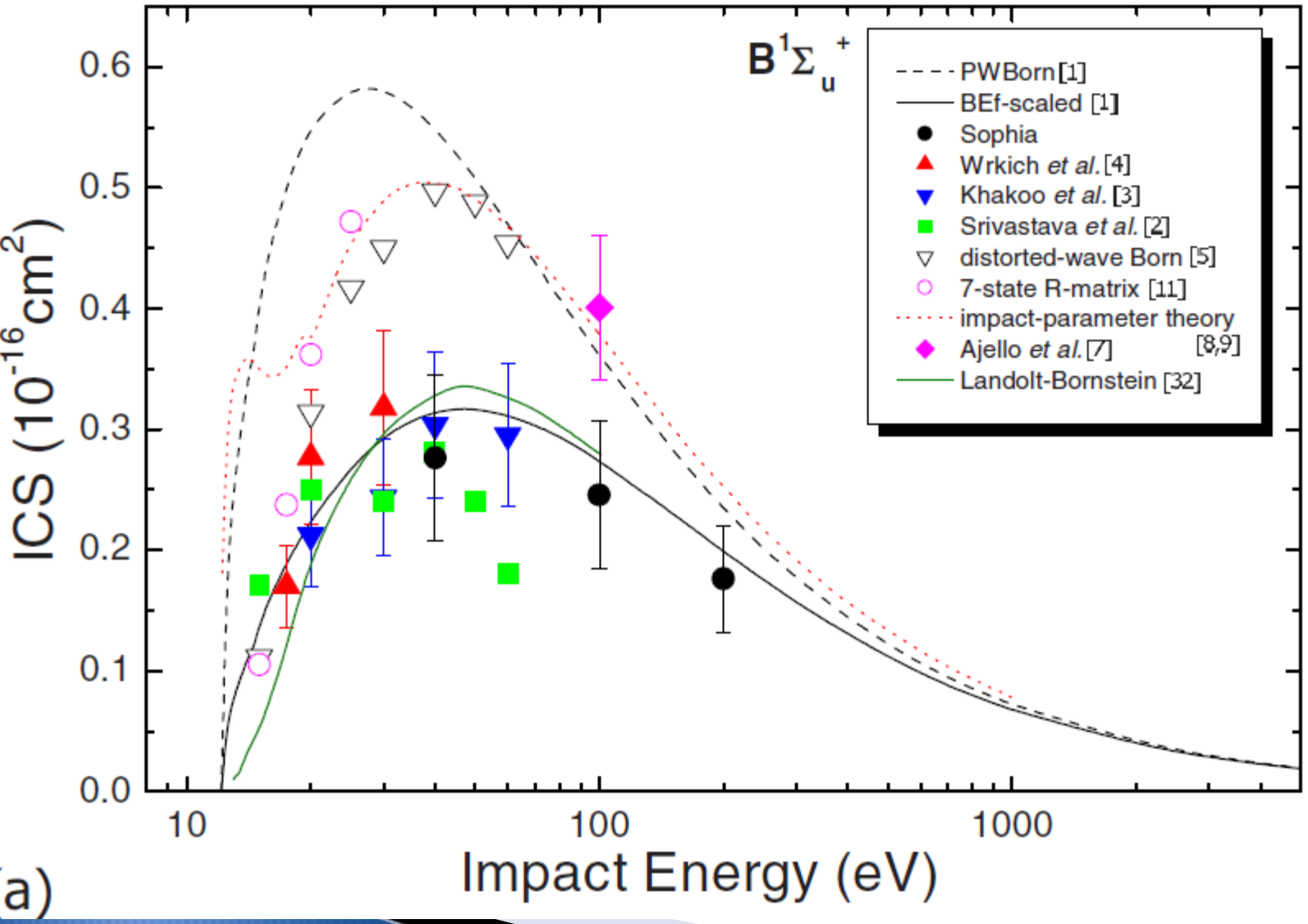
$$Q = \frac{T}{T + B + E} Q_{Born}$$

T: energy of incident electron
B: binding energy of the excited electron
E: excitation energy

Y.-K.Kim, J. Chem. Phys. 126, 064305 (2007)

例題: e + H_2

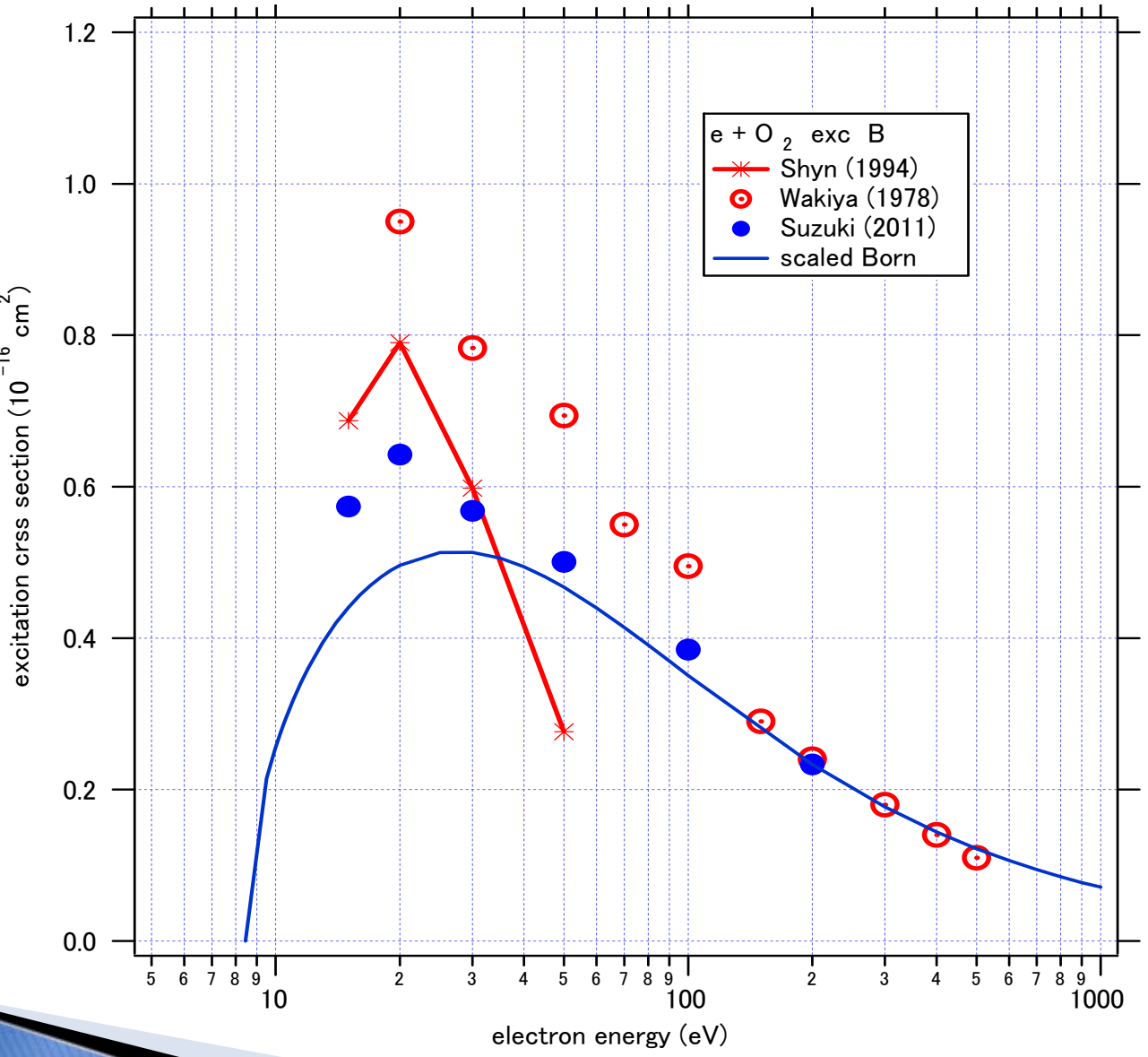
Kato et al., Phys. Rev. A 77, 062708 (2008)



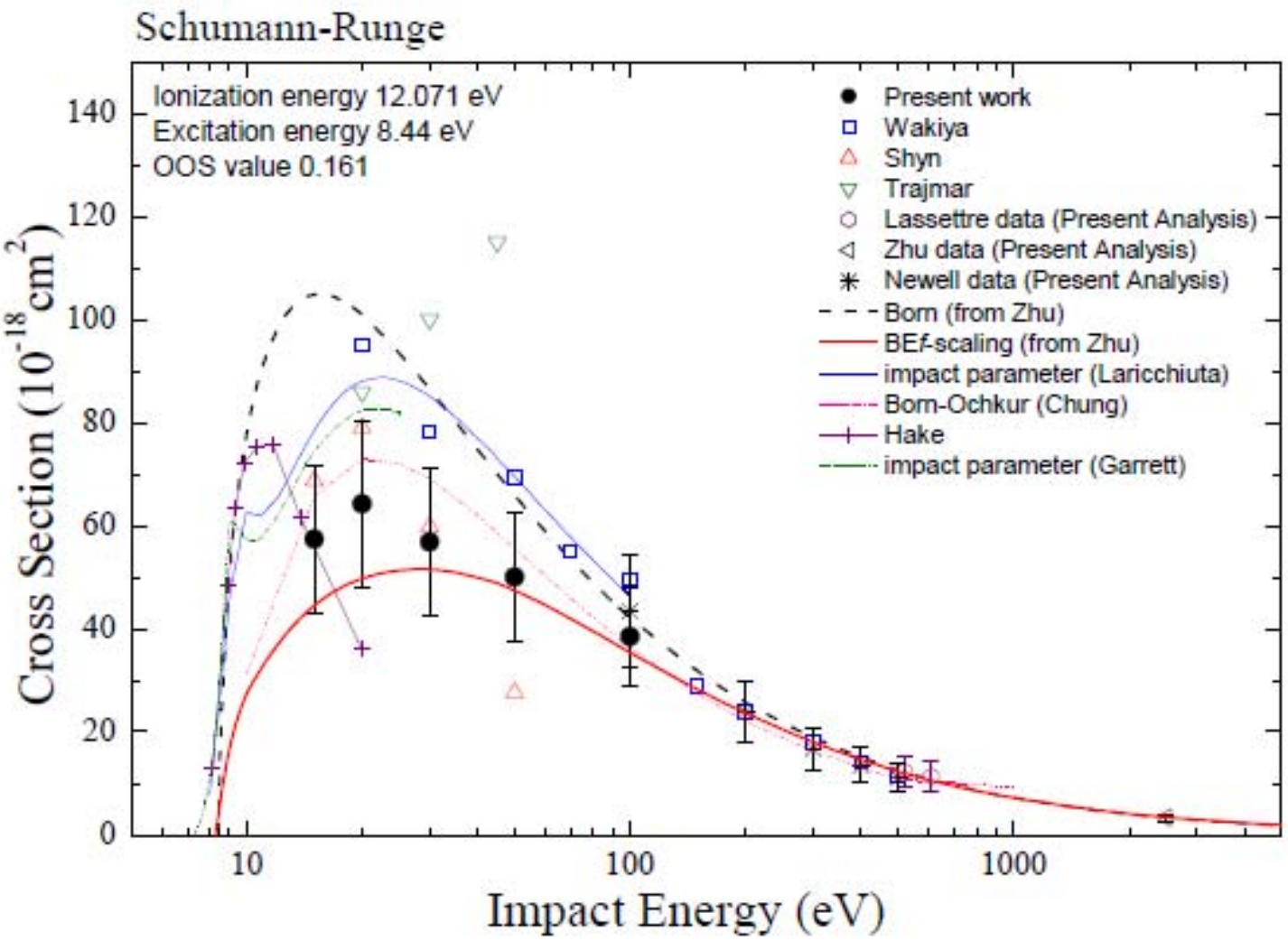
Q_{Born} for O_2

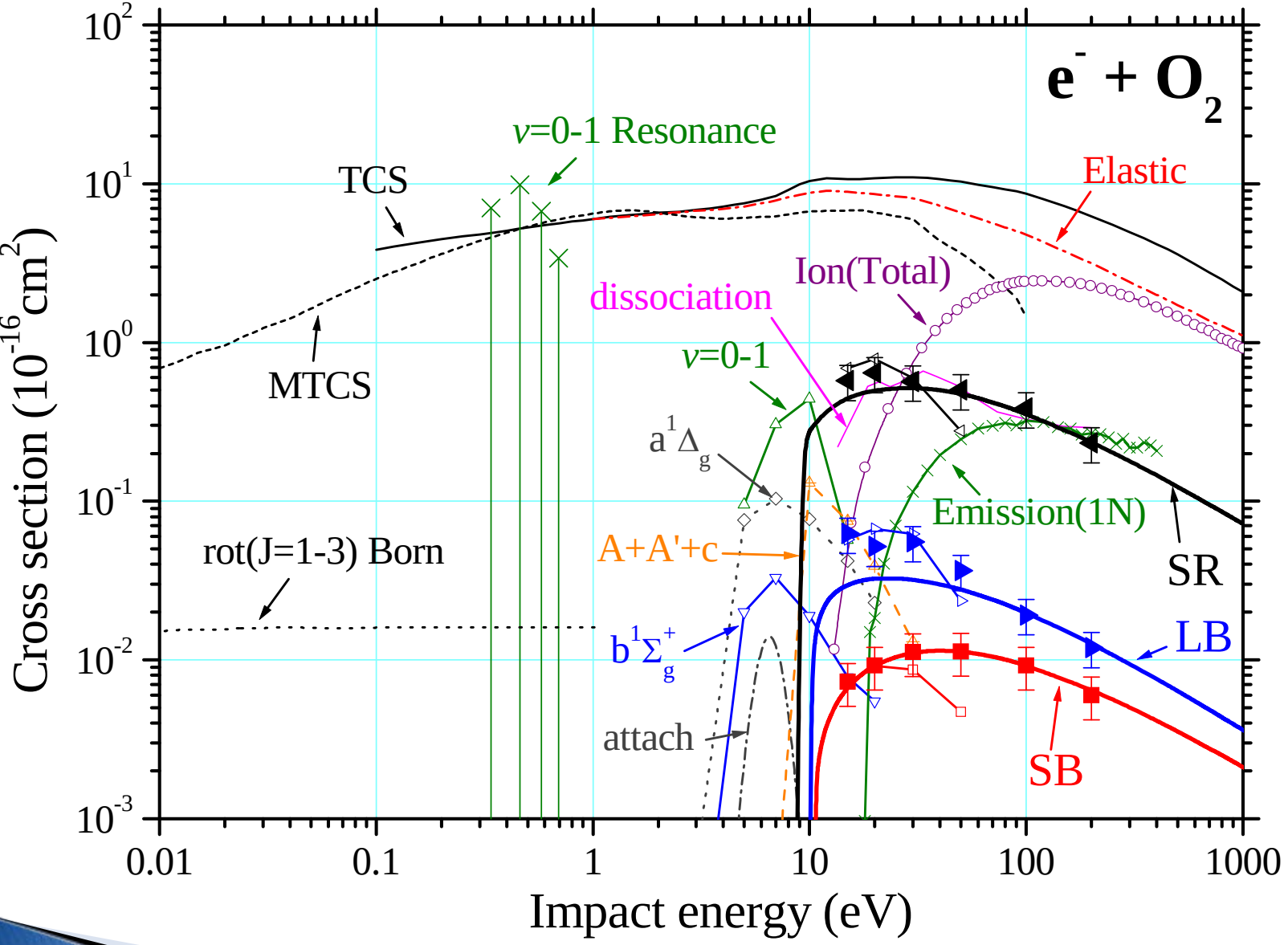
Wei-Qing Xu et al.,
Phys. Rev. A 82, 042716 (2010)

25 keV の電子を使って微分断面積を測定


e + O 2 exc B
Shyn (1994)
Wakiya (1978)
Suzuki (2011)
scaled Born
excitation crss section (10 -16 cm 2)
electron energy (eV)
0.0
0.2
0.4
0.6
0.8
1.0
1.2
10
100
1000

From Suzuki (2010)




e- + O2
v=0-1 Resonance
TCS
Elastic
Ion(Total)
dissociation
v=0-1
MTCS
a1Δg
Emission(1N)
A+A'+c
rot(J=1-3) Born
SR
LB
b1Σg+
attach
SB
Cross section (10-16cm2)
Impact energy (eV)
10^2
10^1
10^0
10^-1
10^-2
10^-3
0.01
0.1
1
10
100
1000

評価の手法（その二）

全散乱断面積　　$Q_T = \Sigma Q$

を使って断面積セットの整合性を確かめる

e + O_2

energy	100 eV	500 ev	1000 eV	uncertainty
total(T)	8.68	3.58	2.08	5 %
elastic(E)	4.78	1.72	1.10	20 %
ionization(I)	2.43	1.46	0.922	5 %
T-(E+I)	**1.47**	**0.40**	**0.06**	
exc	0.41	0.13	0.08	25 %
dissociation	0.33			

cross section in 10^{-16} cm^2

モデリング

高速の荷電粒子と気体の相互作用

放射線作用

惑星大気発光現象（オーロラ等）

あらゆる衝突過程についての情報（断面積）が必要

Nucl. Instr. Meth. A 536, 176 (2005)

Available online at www.sciencedirect.com
SCIENCE DIRECT®
ELSEVIER
Nuclear Instruments and Methods in Physics Research A 536 (2005) 176–188
NUCLEAR INSTRUMENTS & METHODS IN PHYSICS RESEARCH Section A
www.elsevier.com/locate/nima

An approach to Monte Carlo simulation of low-energy electron and photon interactions in air

A. Muñoz[a], J.M. Pérez[a,*], G. García[b], F. Blanco[c]

[a]*Laboratorio General de Electrónica y Automática, Centro de Investigaciones Energéticas Medioambientales y Tecnológicas (CIEMAT), Avenida Complutense 22, 28040 Madrid, Spain*
[b]*Instituto de Matemáticas y Física Fundamental, Consejo Superior de Investigaciones Científicas, Serrano 121, 28006 Madrid, Spain*
[c]*Departamento de Física Atómica, Molecular y Nuclear, Universidad Complutense de Madrid, Avenida Complutense s.n., 28040 Madrid, Spain*

Received 6 July 2004; accepted 13 July 2004
Available online 13 August 2004

$e + O_2, N_2$

(1) 全散乱断面積 Q_T

実験

(2) 弾性散乱 Q_{elas}

計算

(3) 非弾性散乱 Q_{inelas}

$$Q_{inelas} = Q_T - Q_{elas}$$

(4) イオン化 Q_{ion}

$$Q_{ion} = c\, Q_{inelas} \quad c = 0.77$$

(5) 微分断面積

弾性散乱　:　　計算

非弾性散乱　＝　弾性散乱　を仮定

(6)　非弾性散乱におけるエネルギー損失

実験で求めたエネルギー損失スペクトルを基にモデルを作る

弾性散乱断面積の計算

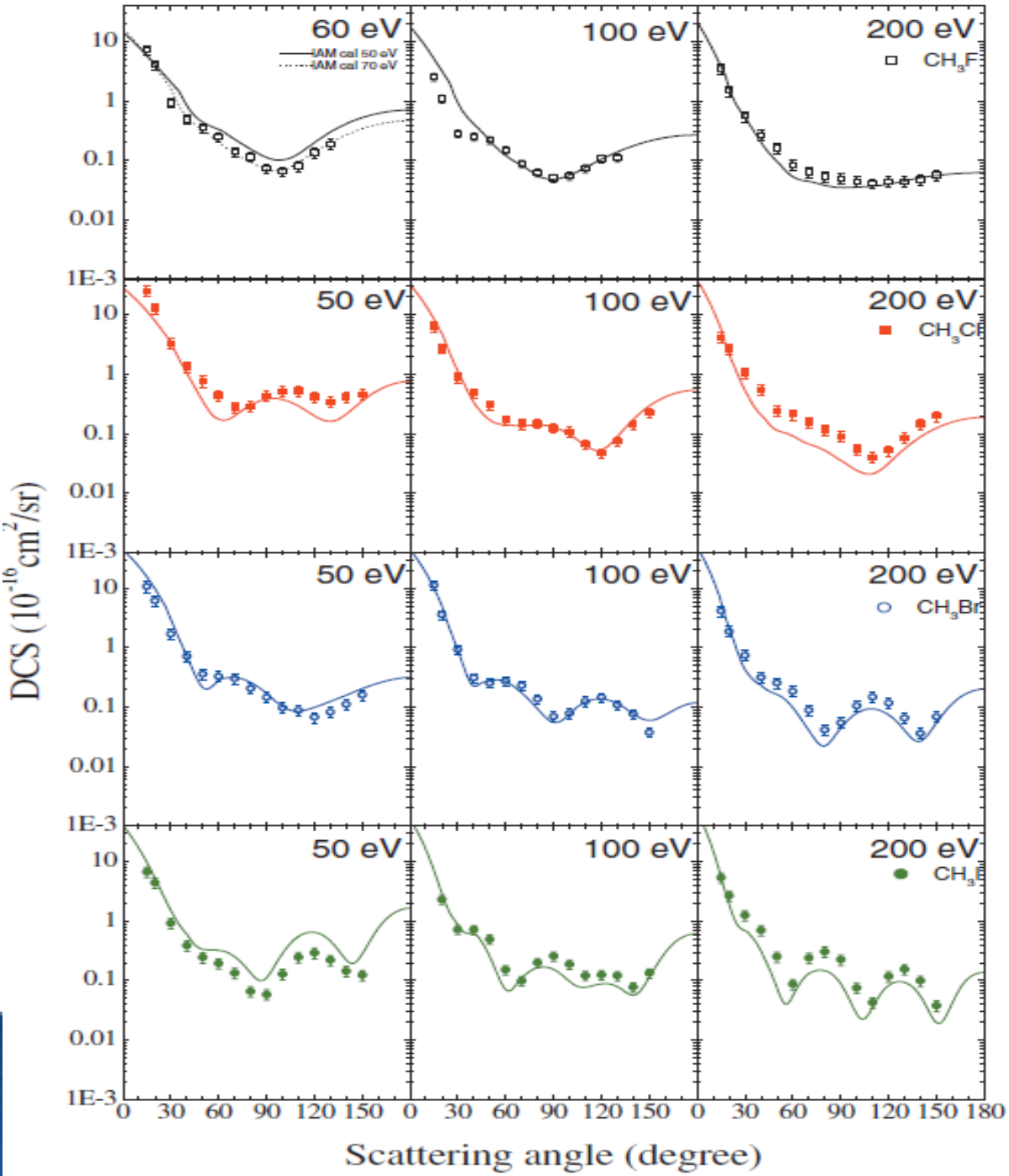
Independent Atom Model (IAM)

散乱振幅　$f^{mol} = \sum f^{atom}$

f^{atom} の計算:

波動関数→　原子ポテンシャル（球対称）

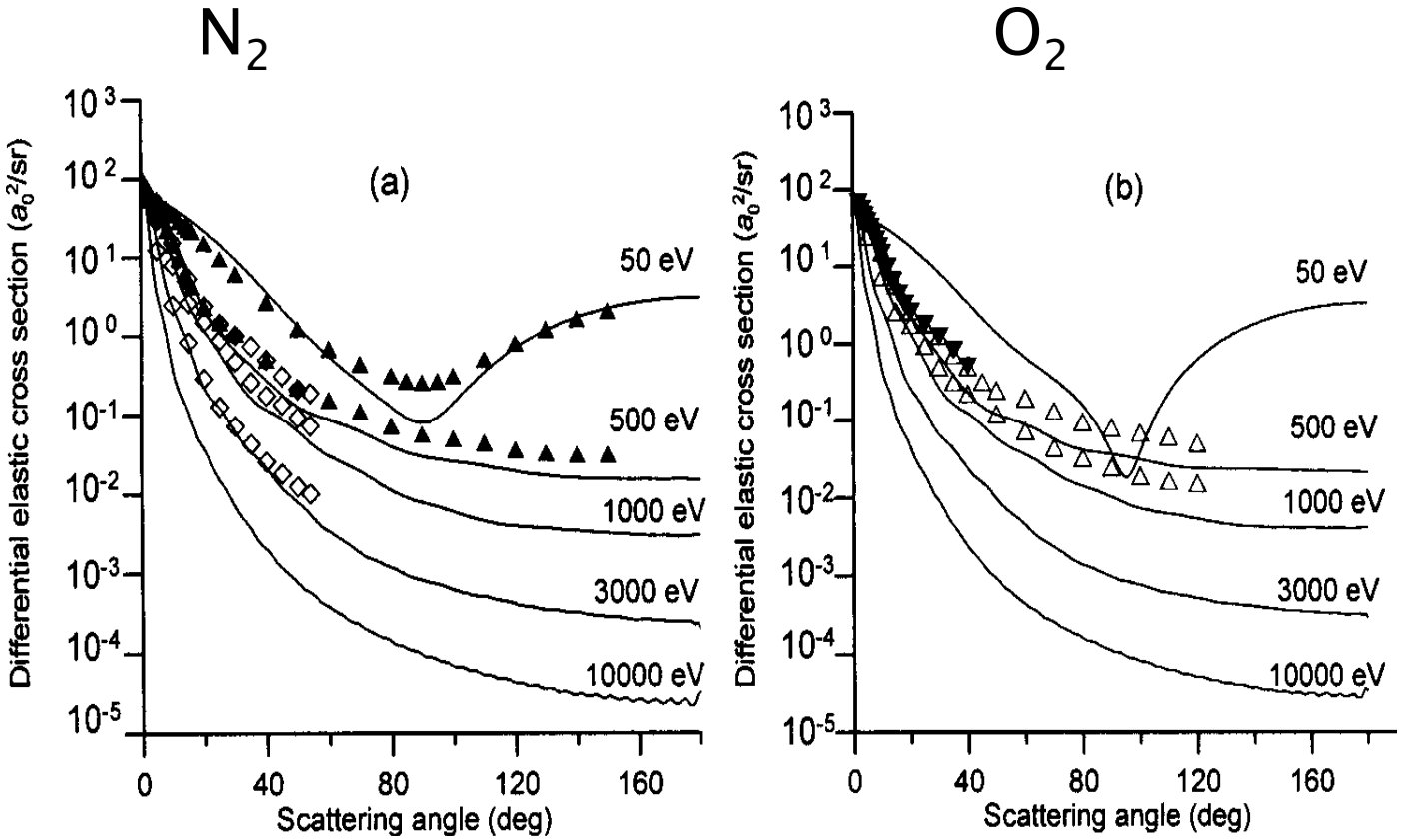
必要に応じて分子形成を考慮する補正を加える



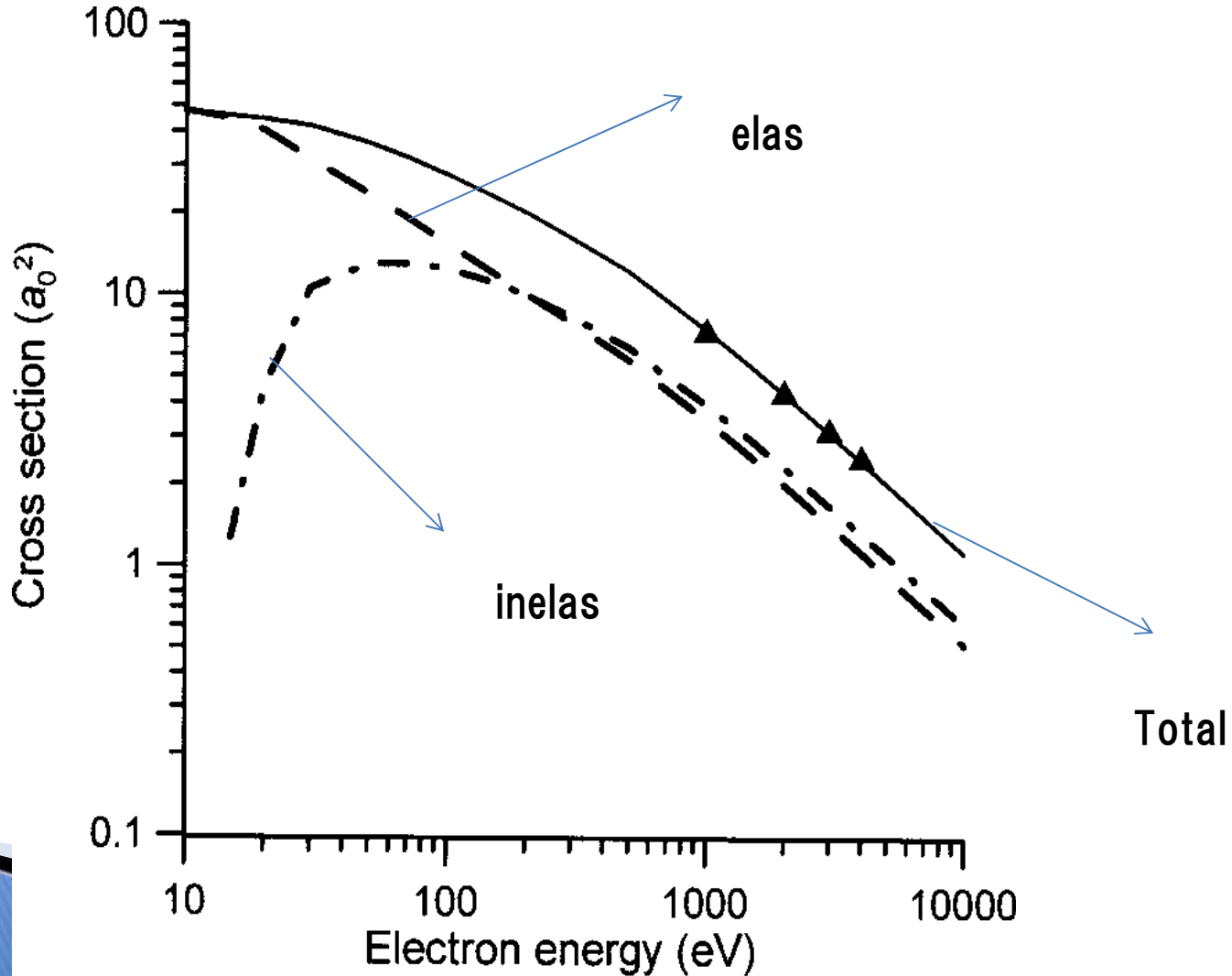
IAM 計算の吟味

Kato et al.
J.Chem.Phys. 132, 074309 (2011)

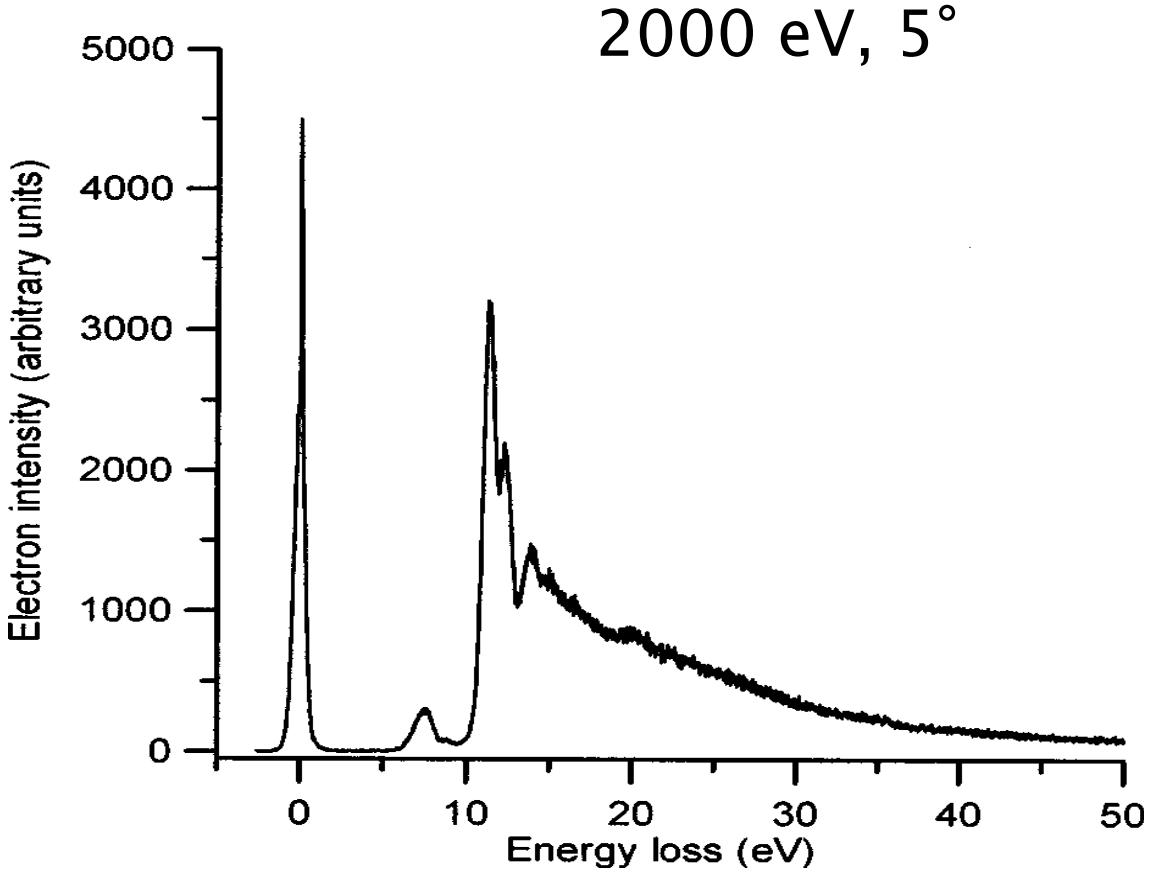
弾性散乱微分断面積


N2
O2
(a)
(b)
Differential elastic cross section (a0²/sr)
Scattering angle (deg)
50 eV
500 eV
1000 eV
3000 eV
10000 eV
10^3
10^2
10^1
10^0
10^-1
10^-2
10^-3
10^-4
10^-5
0
40
80
120
160

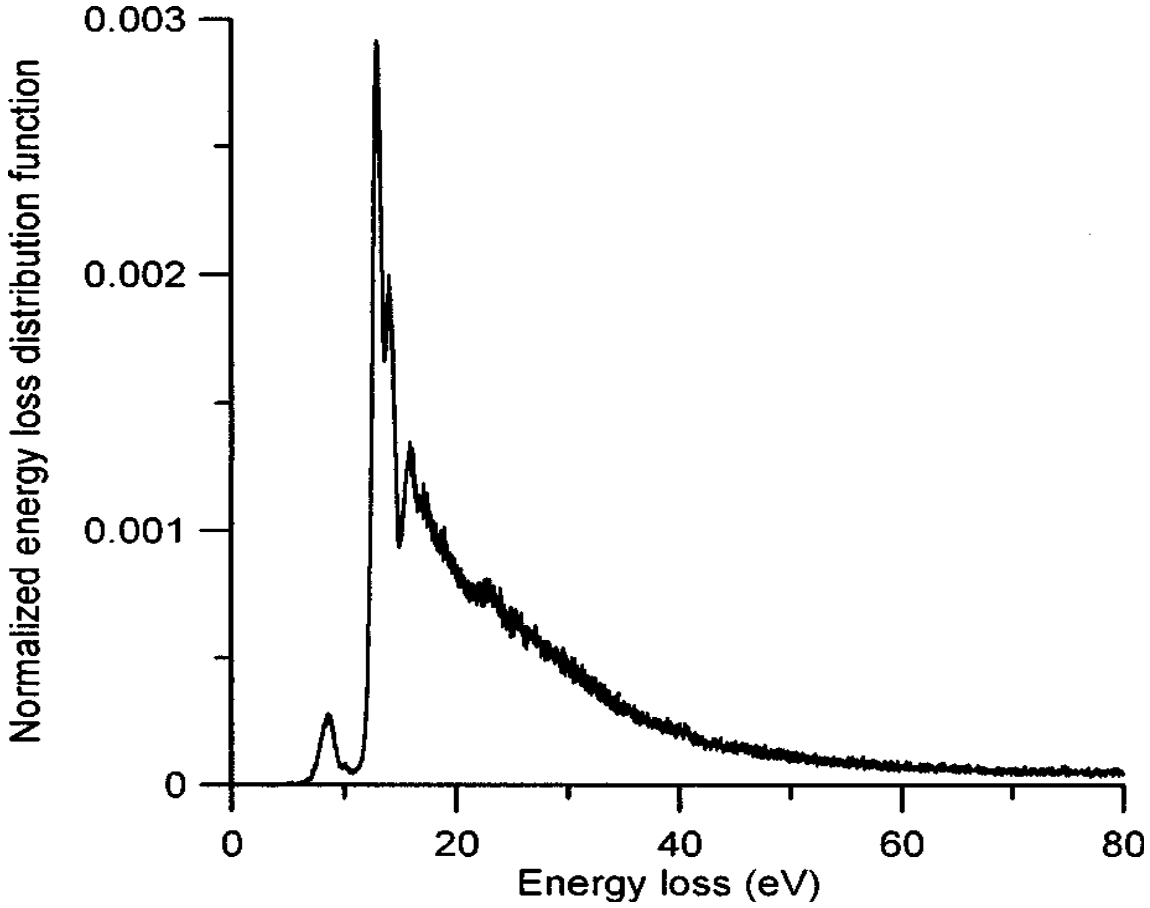
Q_T , Q_{elas} , Q_{inelas}



エネルギー損失スペクトル



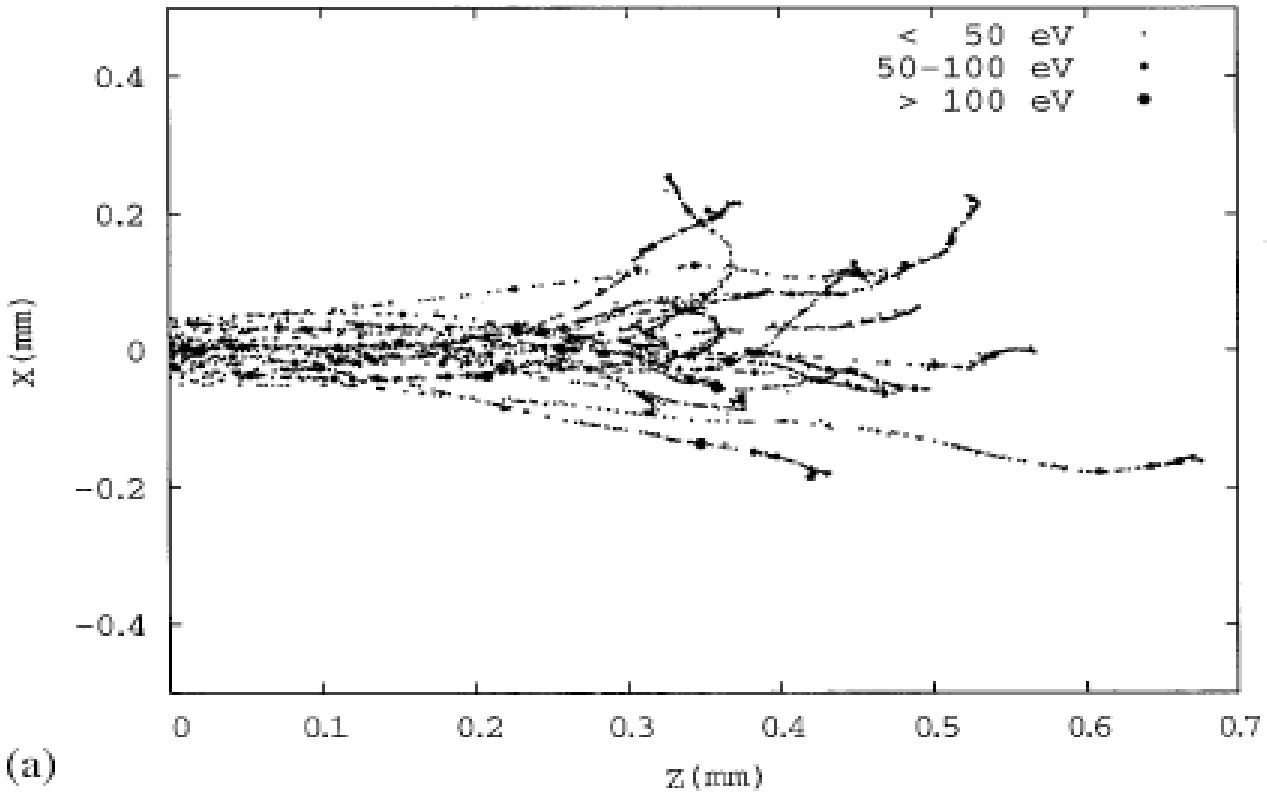
エネルギー損失分布（モデル）



モンテ・カルロ計算

2 keV 電子 → 空気(1気圧)

Energy deposition の分布



$e \rightarrow H_2O$

24th Summer School and International Symposium on the Physics of Ionized Gases IOP Publishing
Journal of Physics: Conference Series **133** (2008) 012002 doi:10.1088/1742-6596/133/1/012002

Energy deposition model based on electron scattering cross section data from water molecules

A.Muñoz[1], J. C. Oller[1], F. Blanco[2], J. D. Gorfinkiel[3], P. Limão-Vieira[4], A. Maira-Vidal[5], M. J. G. Borge[5], O. Tengblad[5], C. Huerga[6], M. Téllez[6] and G. García[7]