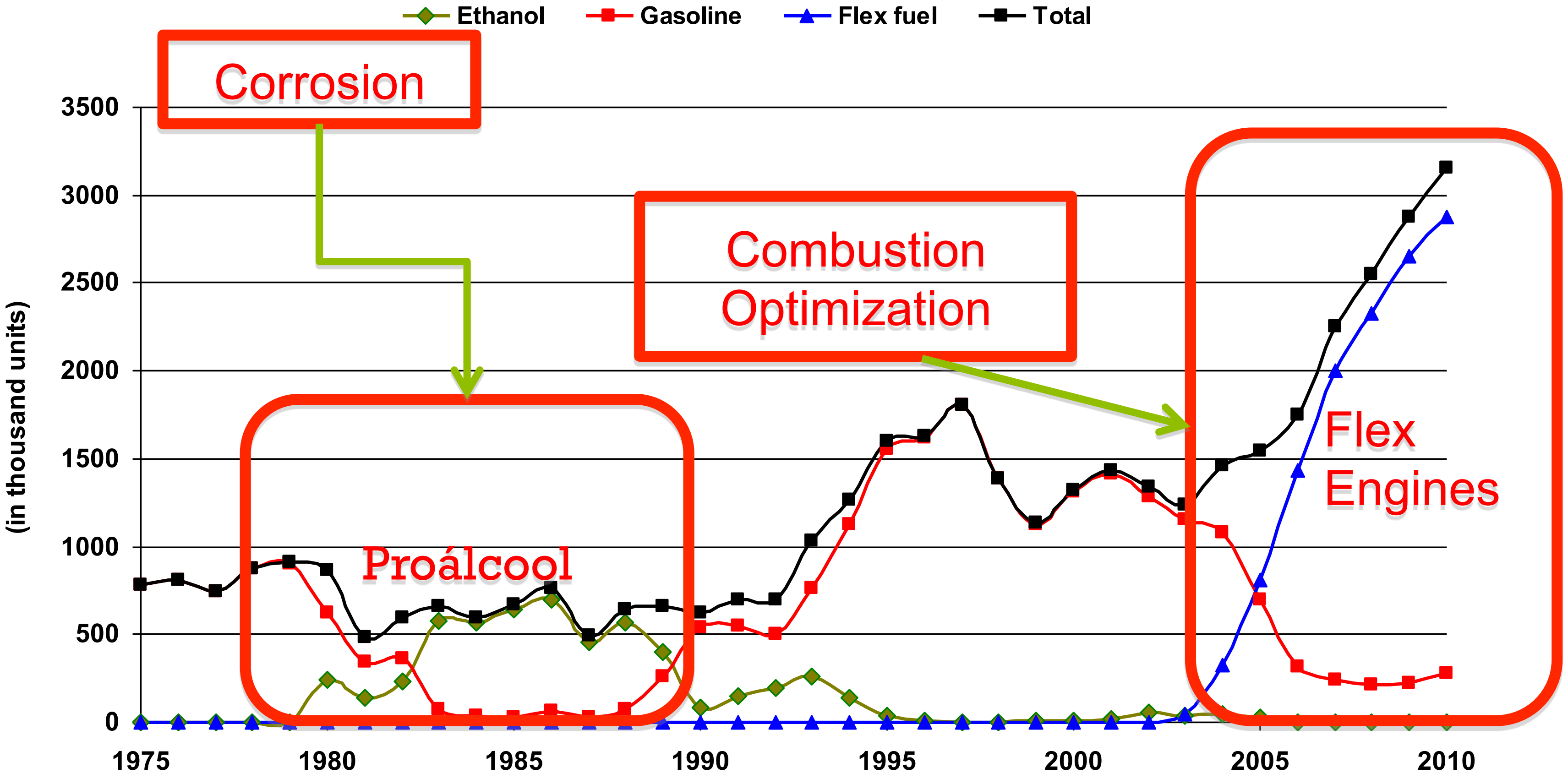
Low energy electron scattering data for chemical plasma treatment of biomass

by

Marco A. P. Lima
Unicamp

Motivation I: large scale use of ethanol in engines



Corrosion

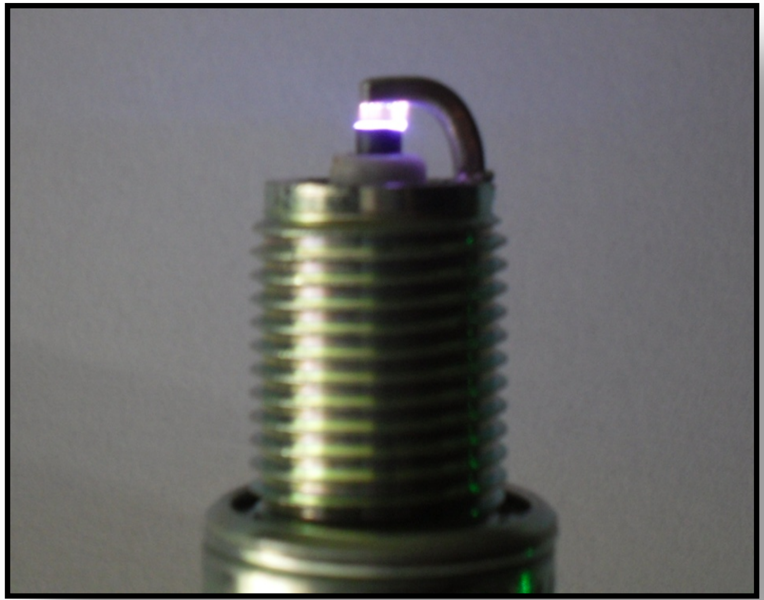
Combustion Optimization

Proálcool

Flex Engines

Brazilian Sales of light fleet Vehicles (1975-2010)

Ethanol as Fuel: Plasma Ignition for Vehicle Engines



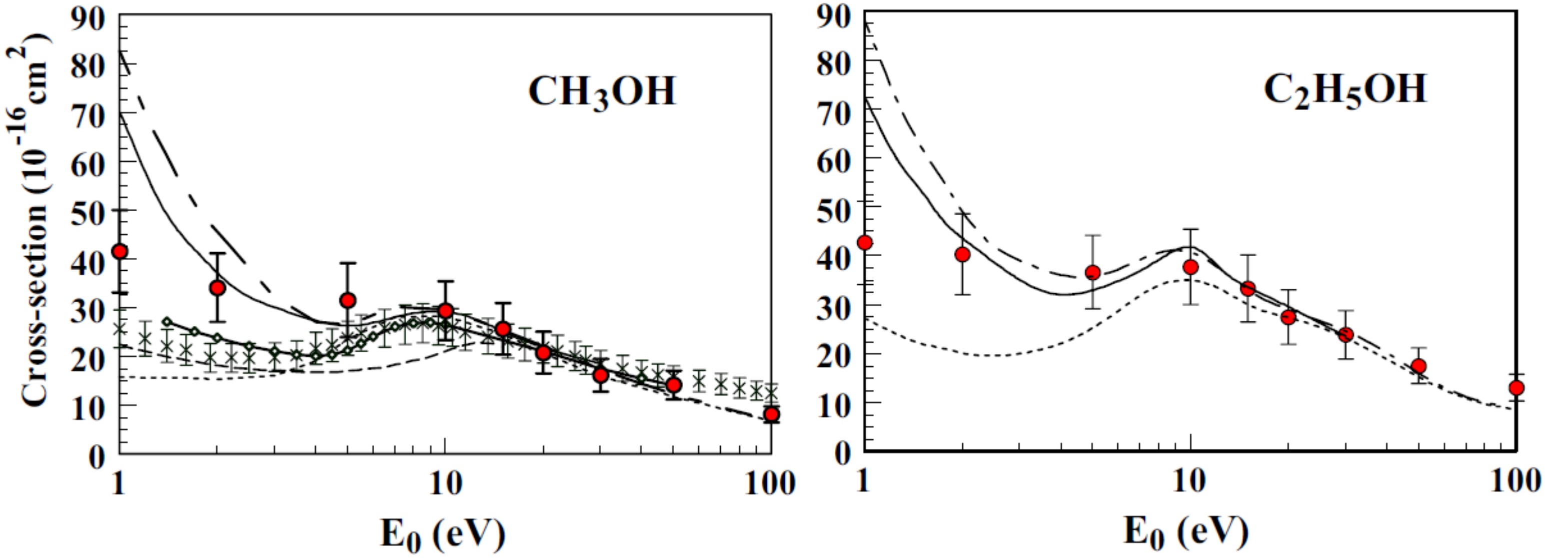
Theoretical support for an application project working on:

- Investigation of processes occurring during the ignition of plasma and its consequences in post-discharge for an internal combustion engine;

- The proper parameters to be applied in cars that operate on "poor mixtures" reducing pollutants released into the atmosphere, especially considering the spark plug discharge.

Low-energy electron scattering from methanol and ethanol

PHYSICAL REVIEW A **77**, 042705 (2008)

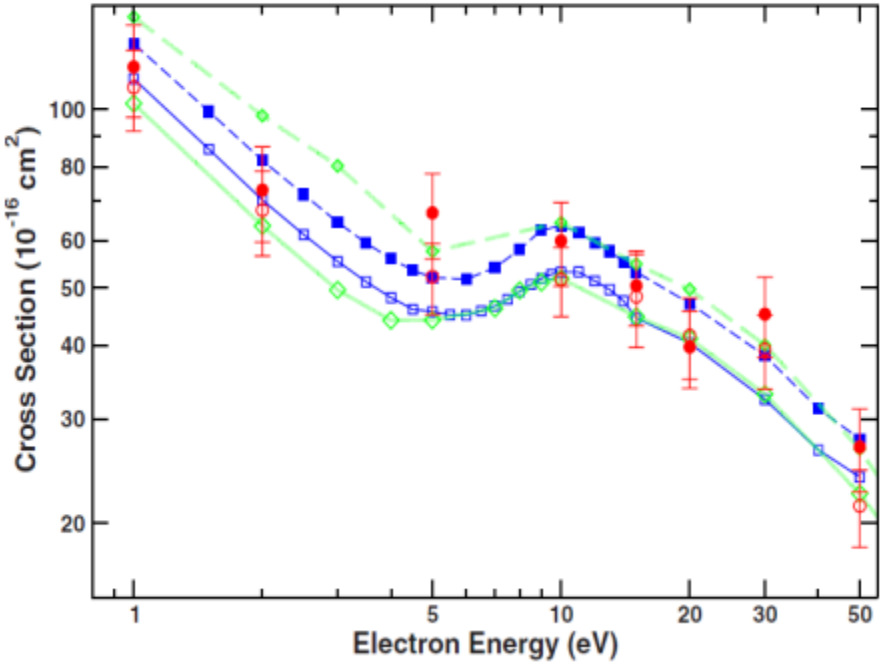


Integral elastic scattering cross sections for CH$_3$OH. Legend: ●: present experiment; ——-—: SMCPP SEP; —: SMC SEP; ---- (short dashes): SMC SE which is similar to SMCPP SE; and ---- (long dashes): *R*-matrix ICSs of Bouchiha *et al.* (without Born correction) [10]. × Total cross section measurements of Szmytkowski and Krzysztofowicz [24] and —◆— of Schmieder [22]. ----- (short dashes) are from the SMCPP SE which is similar to SMC SE.

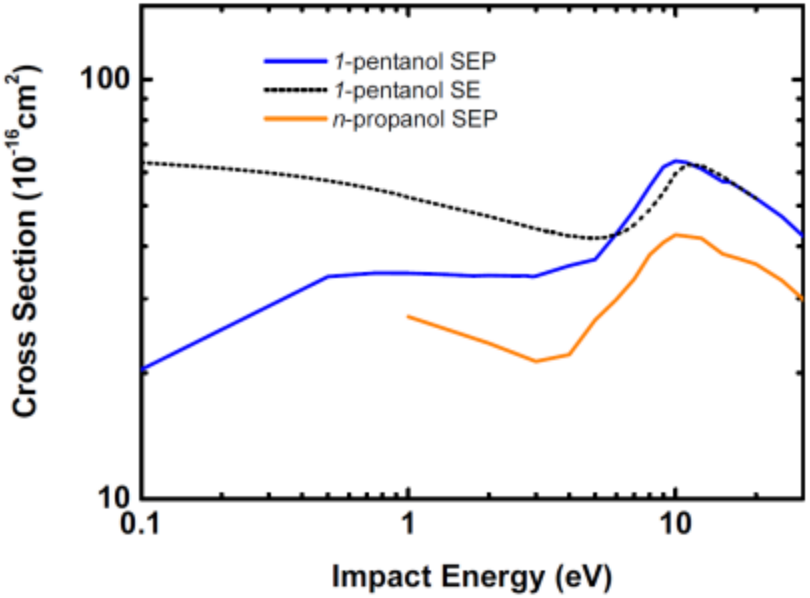
NSF/CNPq project (experiments from Morty Khakoo's group)

Elastic scattering of slow electrons by *n*-propanol and *n*-butanol

PHYSICAL REVIEW A **78**, 062714 (2008)



Electron scattering of slow electrons by *1*-pentanol (a drop in fuel)



Integral elastic cross sections for electron collisions with *n*-propanol and *n*-butanol. Red circles are experimental values, thin blue lines with squares results from all-electron calculations, and thick green lines with diamonds results from pseudopotential calculations. Open symbols and solid lines are propanol data; solid symbols and dashed lines are butanol data.

NSF/CNPq project (experiments from Morty Khakoo's group)

Motivation II: large scale production of ethanol

A sugarcane industry of Sugar/Ethanol/Bioeletricity

Motivation II: large scale production of ethanol

Biomass: a source of energy and carbon

Motivation II: large scale production of ethanol

Biomass: a source of energy and carbon

Motivation II: large scale production of ethanol

Biomass: a source of energy and carbon

Motivation II: large scale production of ethanol

First generation ethanol: crushing the cane for the juice

Motivation II: large scale production of ethanol

Bagasse piles
at the mill.

2nd generation
ethanol?
Other high value
bioproducts?

Biomass: a source of energy and carbon

Funding Motivation

FAPESP BIOEN FAPESP

- Feedstock, processing, green chemistry, engines, sustainability

- 300+ scientists (50 from abroad); 600+ graduate students

- Value awarded 2009-2012:
  US$ 45 million (FAPESP);
  US$ 28 million (State Government);
  US$ 5 million (industry);
  US$ 28 million (Universities)

BNDES FINEP AGÊNCIA BRASILEIRA DA INOVAÇÃO

- 35 industrial business plans (2nd generation ethanol; new products for sugarcane; gasification) approved will result in a potential investment of BRL 3.1 billion (~US$ 1.5 billion)

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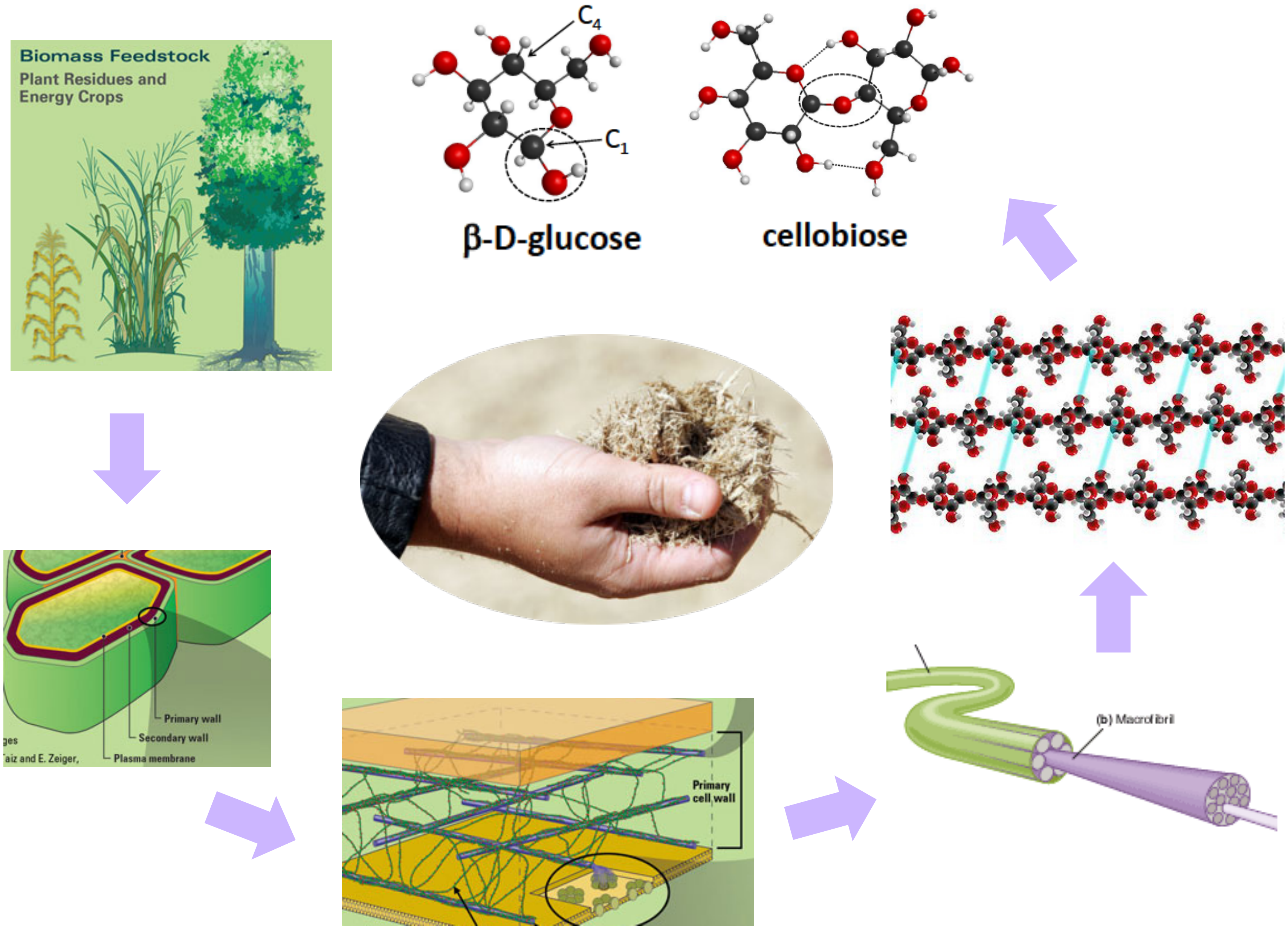
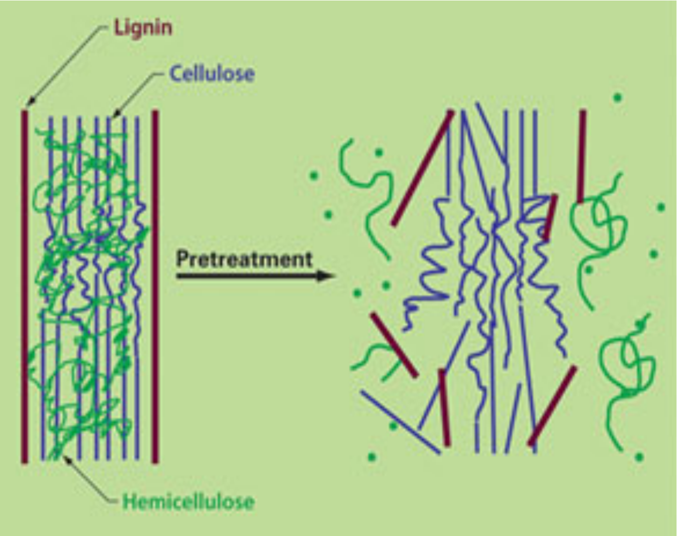
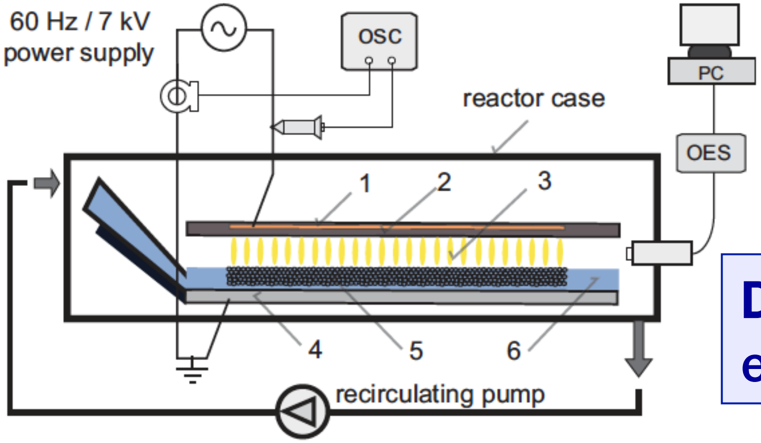
Biomass is Made Up with Fermentable Sugars

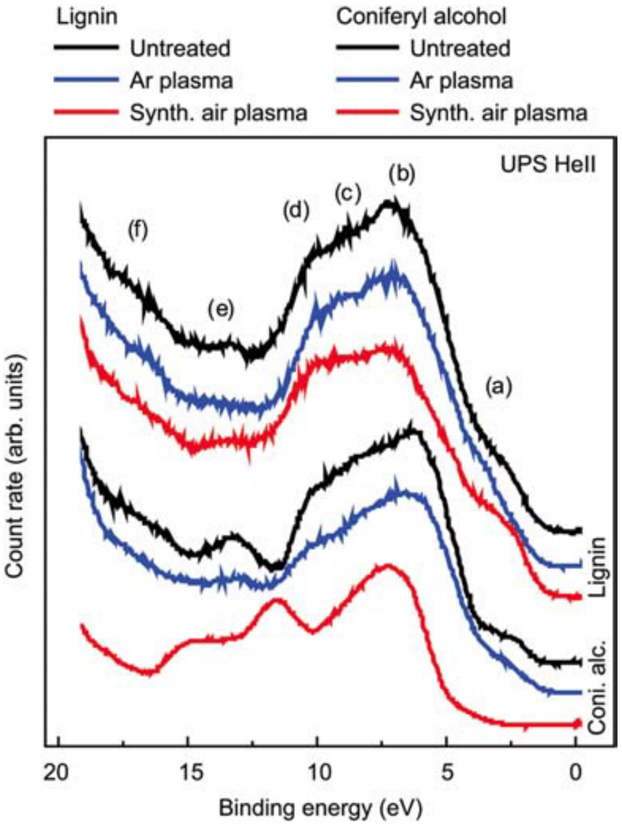


Lignocellulose is Resistant to Hydrolysis



Pretreatment: bio- and physical-chemical processes to expose the cellulose fibers



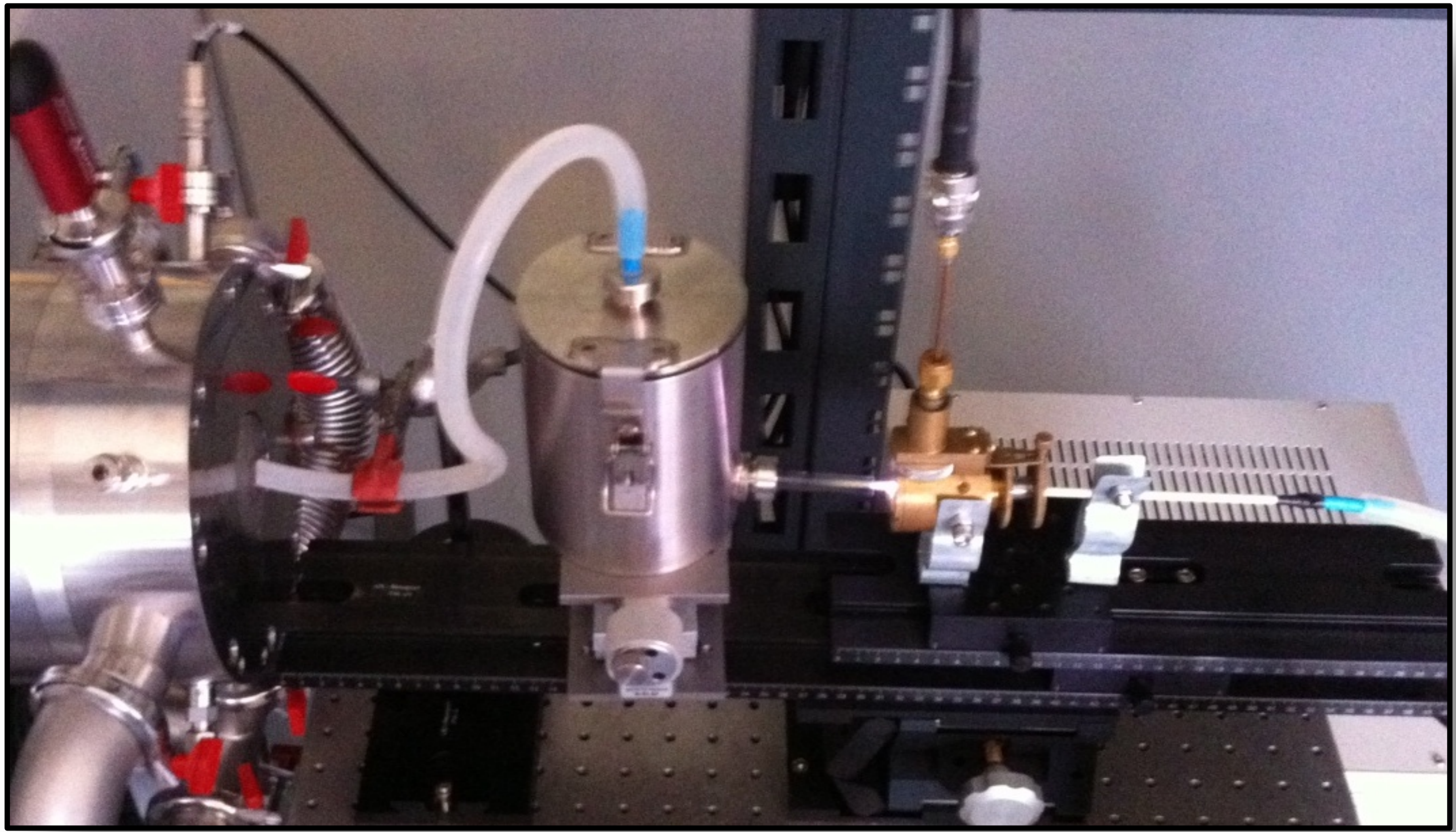


Lothar Klarhöfer[1], Wolfgang Viöl[2,3,*] and Wolfgang Maus-Friedrichs[1]

Holzforschung, Vol. 64, pp. 331–336, 2010

Dielectric Barrier Discharge (DBD): electron flux on substrate ~10^8 cm^{-2} s^{-1}

Sugarcane Bagasse Plasma Pretreatment



Treatment conditions

- ~ 25 g of dry sugarcane bagasse (50% moisture) – milled at 500μm
- Gas flow Mixture: 95% Ar (1.9 SLM) and 5% O_2 (0.1 SML)
- $\Delta t_{treatment}$ = 3h

Biomass Chemical Analysis

Lignin concentration (%) of raw bagasse and samples related to plasma torch treatment and washing procedure by water and NaOH 1% solution at room temperature.

Samples	Soluble Lignin (%)	Insoluble Lignin (%)	Total of Lignin remaining (%)
raw bagasse	1.58 ±0.01	20.3 ± 0.1	21.9 ± 0.1
Washed by H_2O	2.4 ± 0.9	21.4 ± 0.9	23.8 ± 0.9
Washed by NaOH 1%	**1.3 ± 0.9**	**12.6 ± 0.9**	**13.9 ± 0.9**

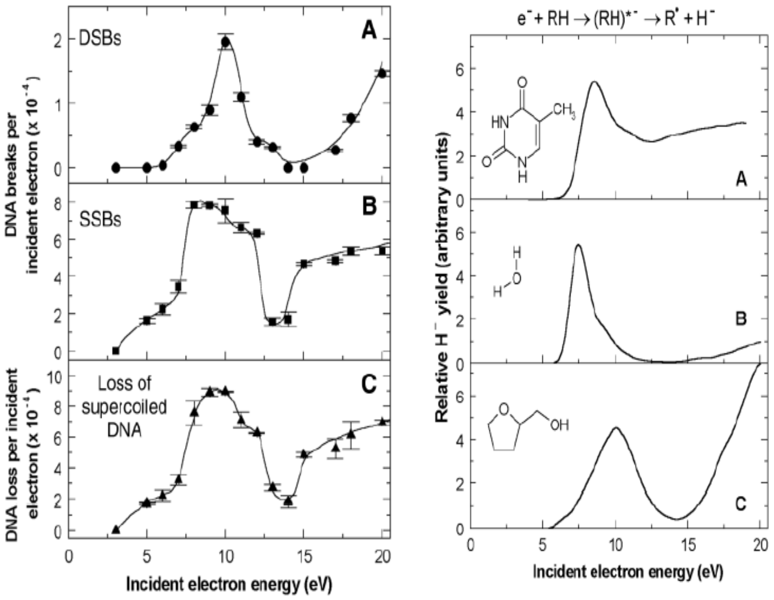
About 40% of original lignin was removed!!!

Jayr Amorim, Carlos Oliveira, Jorge A. Souza-Correa, Marco A. Ridenti
Plasma Process. Polym. 2013, DOI: 10.1002/ppap.201200158

Electron-Induced Damage to Biomolecules

Resonant Formation of DNA Strand Breaks by Low-Energy (3 to 20 eV) Electrons

Badia Boudaïffa, Pierre Cloutier, Darel Hunting,
Michael A. Huels,* Léon Sanche



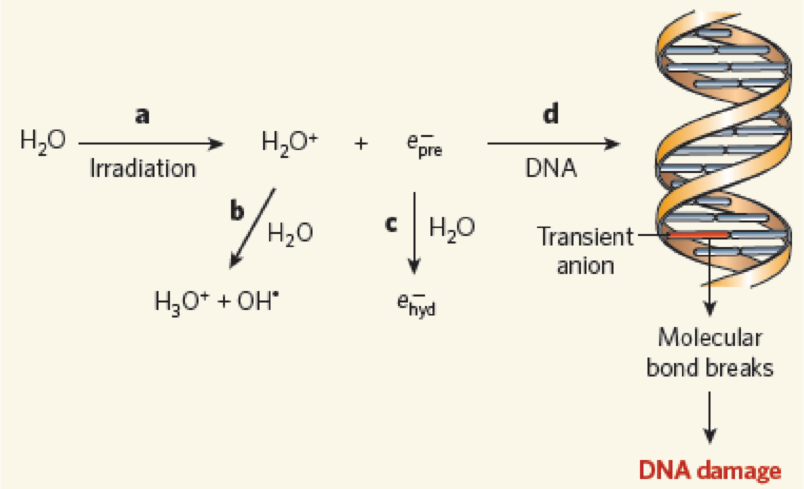
Science, **287** 1658 (2000)

BIOLOGICAL CHEMISTRY

Beyond radical thinking

Léon Sanche

Radiation-induced DNA damage has been attributed to hydroxyl radicals, which form when water absorbs high-energy photons or charged particles. But another product of water's radiolysis might be the real culprit.



Sanche, Nature **461**, 358 (2009)

J|A|C|S COMMUNICATIONS

Chun-Rong Wang, Jenny Nguyen, and Qing-Bin Lu*

J. AM. CHEM. SOC. 2009, *131*, 11320–11322

Electron scattering by Molecules

DISCHARGE ENVIROMENTS

Basic Science →

Natural Phenomena	Aurora Borealis
Astrophysics	Planetary Atmospheres
Biology	DNA dissociation
Quantum Optics	Molecular Lasers

Applications →

- Control of pollution
- Ozone destruction
- Surface treatment

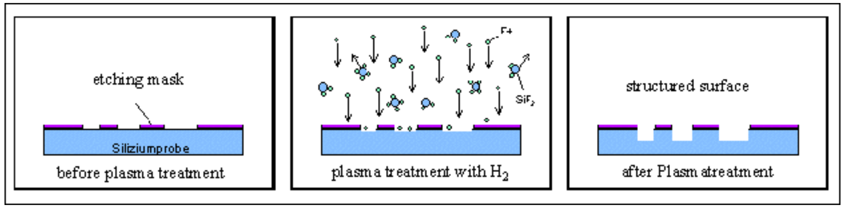
Surface treatment with Plasmas

Plasma
Processing
Gases

Several Industry Applications

Production
of reactive
species

ETCHING, DIAMANTIZATION,
POLIMERIZATION, NITRIDING,
CLEANING, and others



IMPROVEMENT NEEDS MODELING
AND MODELING NEEDS DATA

Electron collision
data: cross
sections for

Elastic
Inelastic: electronic, rotational and vibrational excitation
Ionization
Dissociation

Academic Motivation

➡ Scientific Challenge: To obtain reasonable results it is necessary to learn how to control APPROXIMATIONS in many-body problems

Electron Molecule Scattering

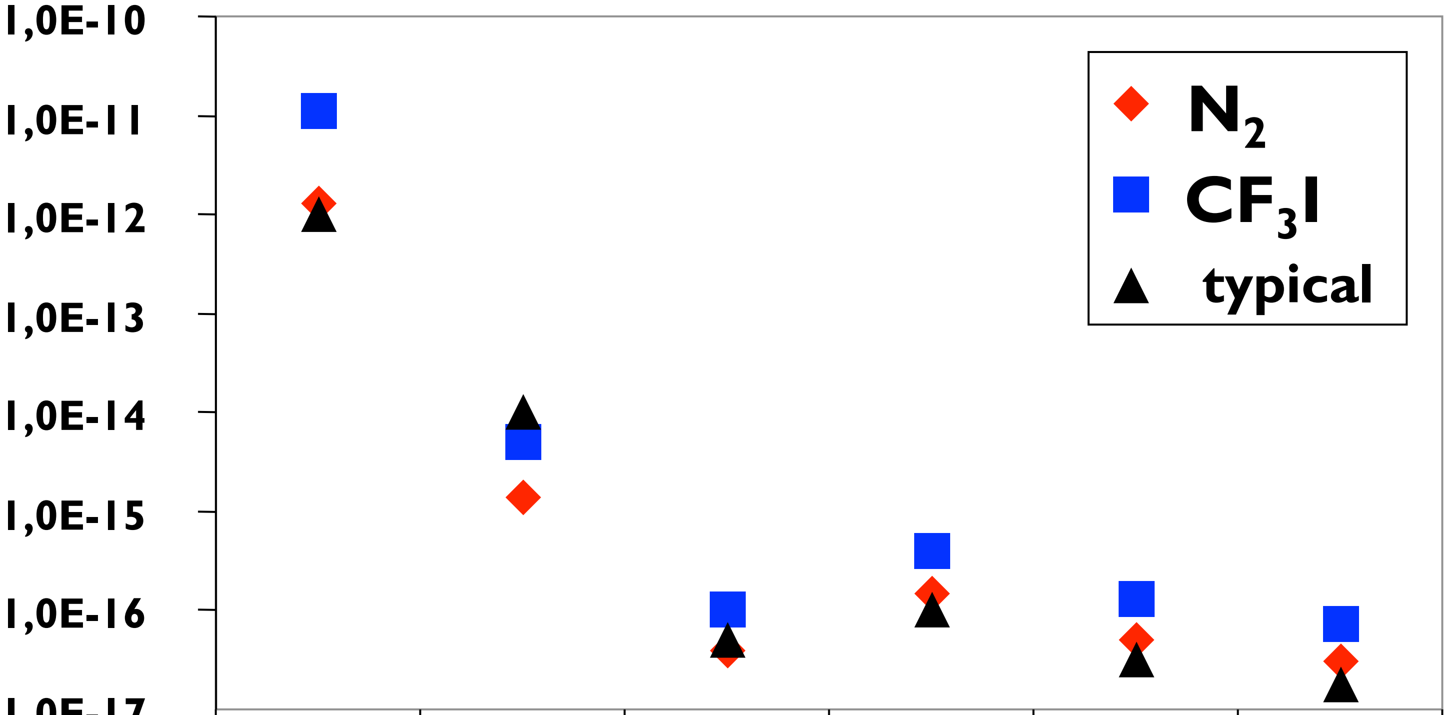
THE COLLISION CAN BE

Elastic

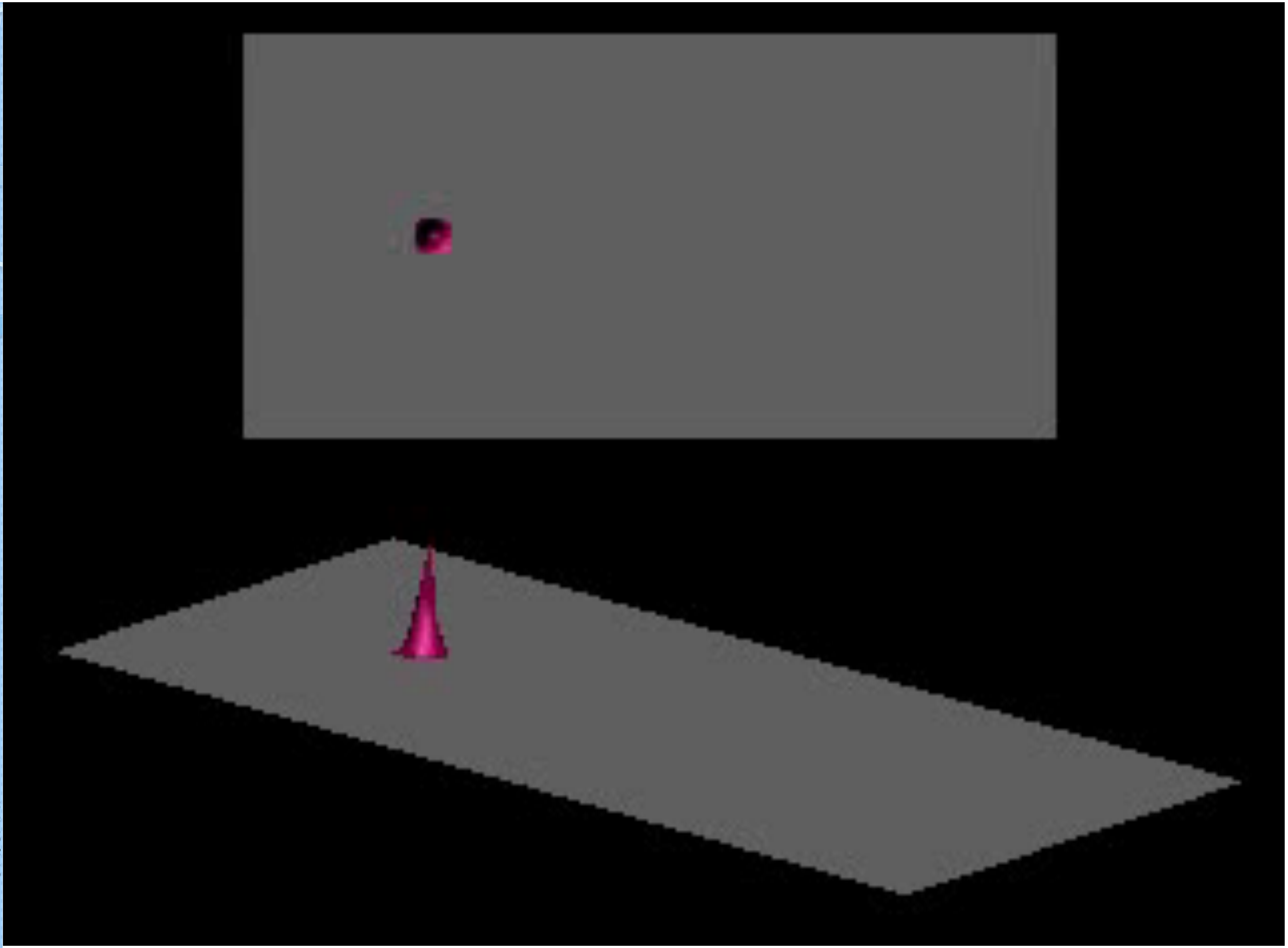
Inelastic

Excitation	Dissociation	Ionization
Rotational	Direct (vibrational excitation)	
Vibrational	Via electronic excitations	
Electronic	Via ressonance (with e without Attachment)	

Typical times (in seconds)

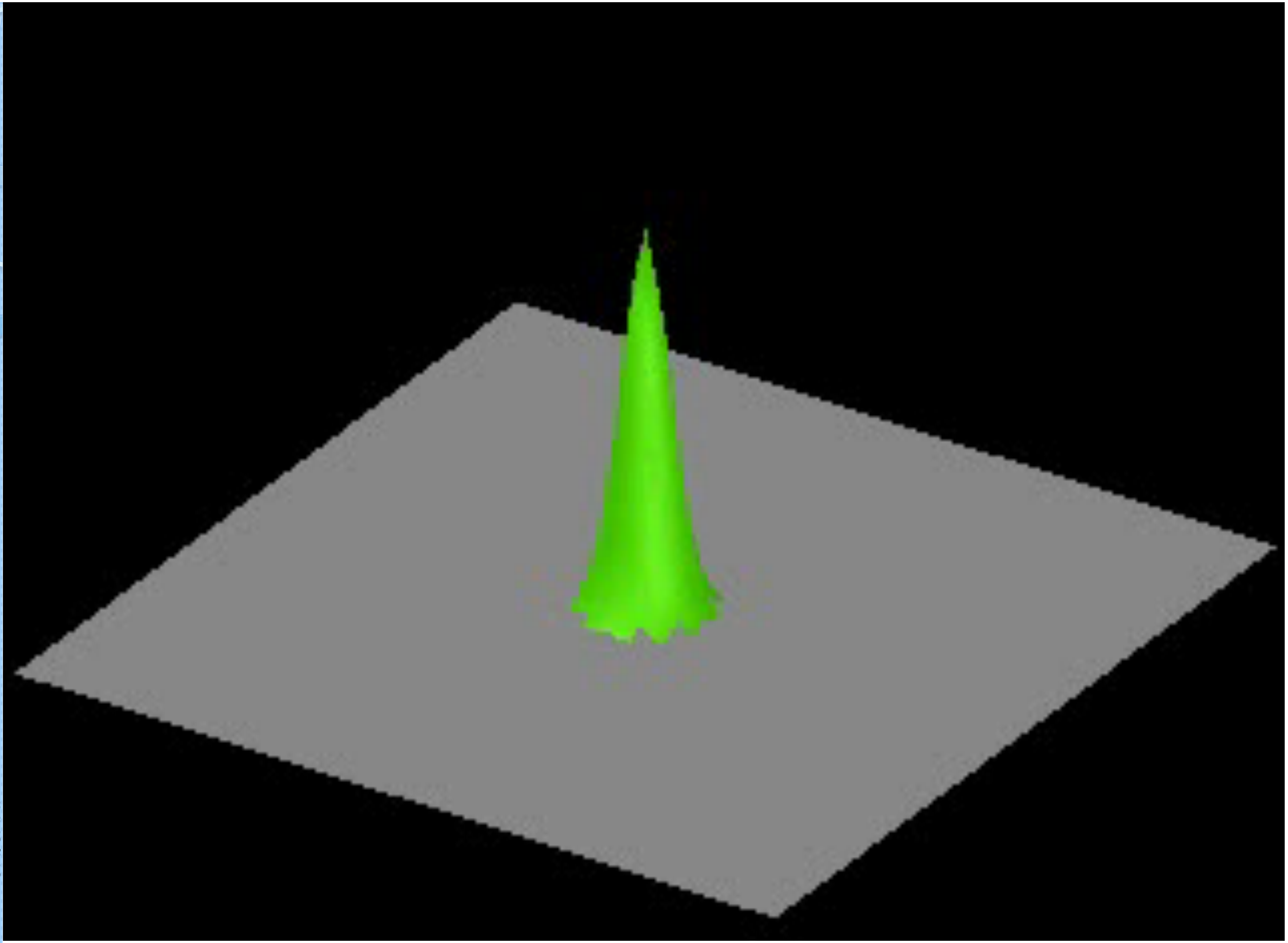


	Rotation	Vibration	Electronic Excitation	Collision ($1eV-20a_0$)	Collision ($10eV-7a_0$)	Collision ($30eV-4a_0$)
◆ N_2	1,30E-12	1,40E-15	4,00E-17	1,50E-16	5,00E-17	3,00E-17
■ CF_3I	1,10E-11	5,00E-15	1,00E-16	4,00E-16	1,30E-16	7,30E-17
▲ Typical	1,00E-12	1,00E-14	5,00E-17	1,00E-16	3,20E-17	1,80E-17



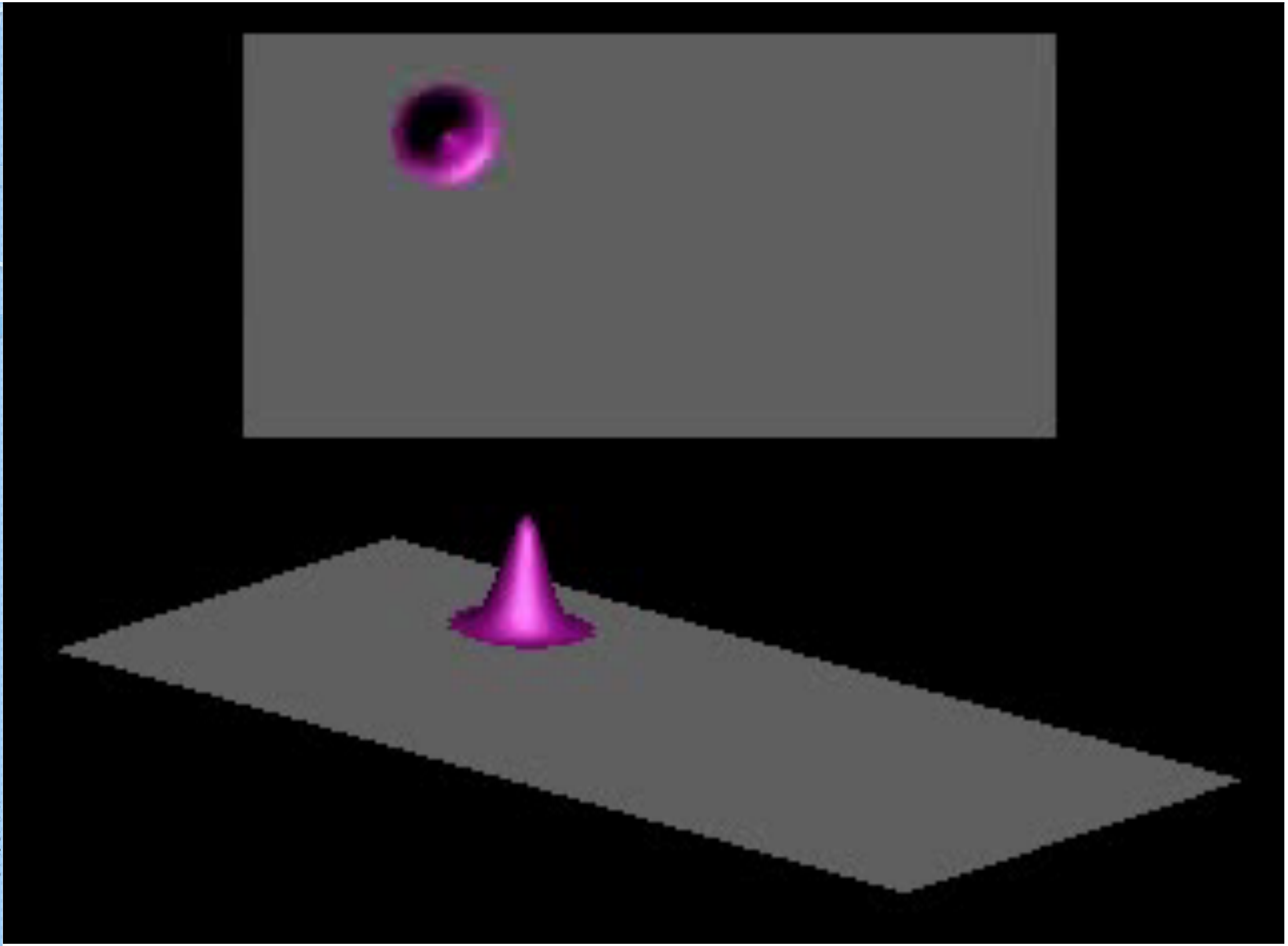
Free Particle

To see this animations, visit: **http://www.embd.be/quantummechanics/**



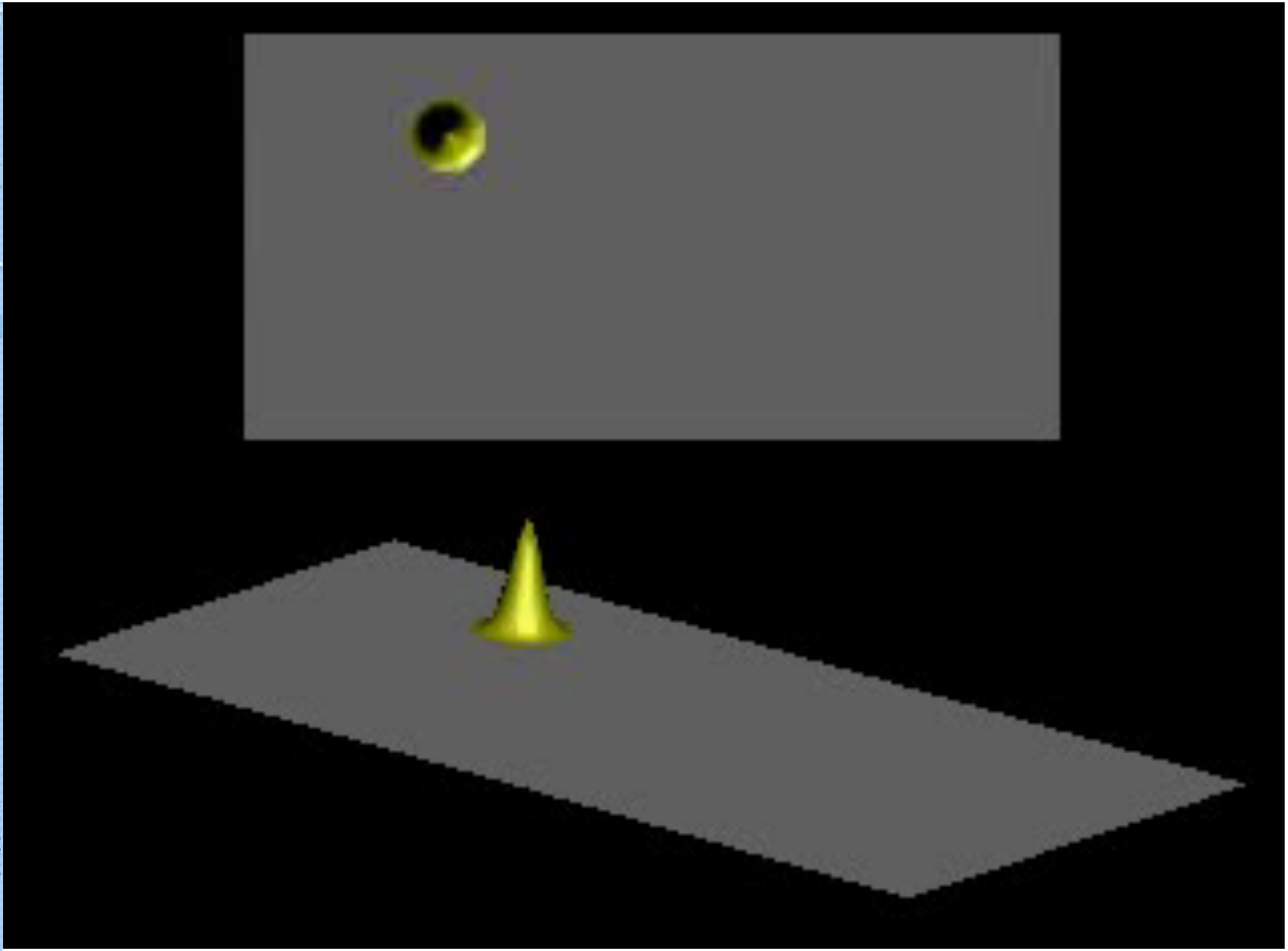
Particle in a box

To see this animations, visit: **http://www.embd.be/quantummechanics/**



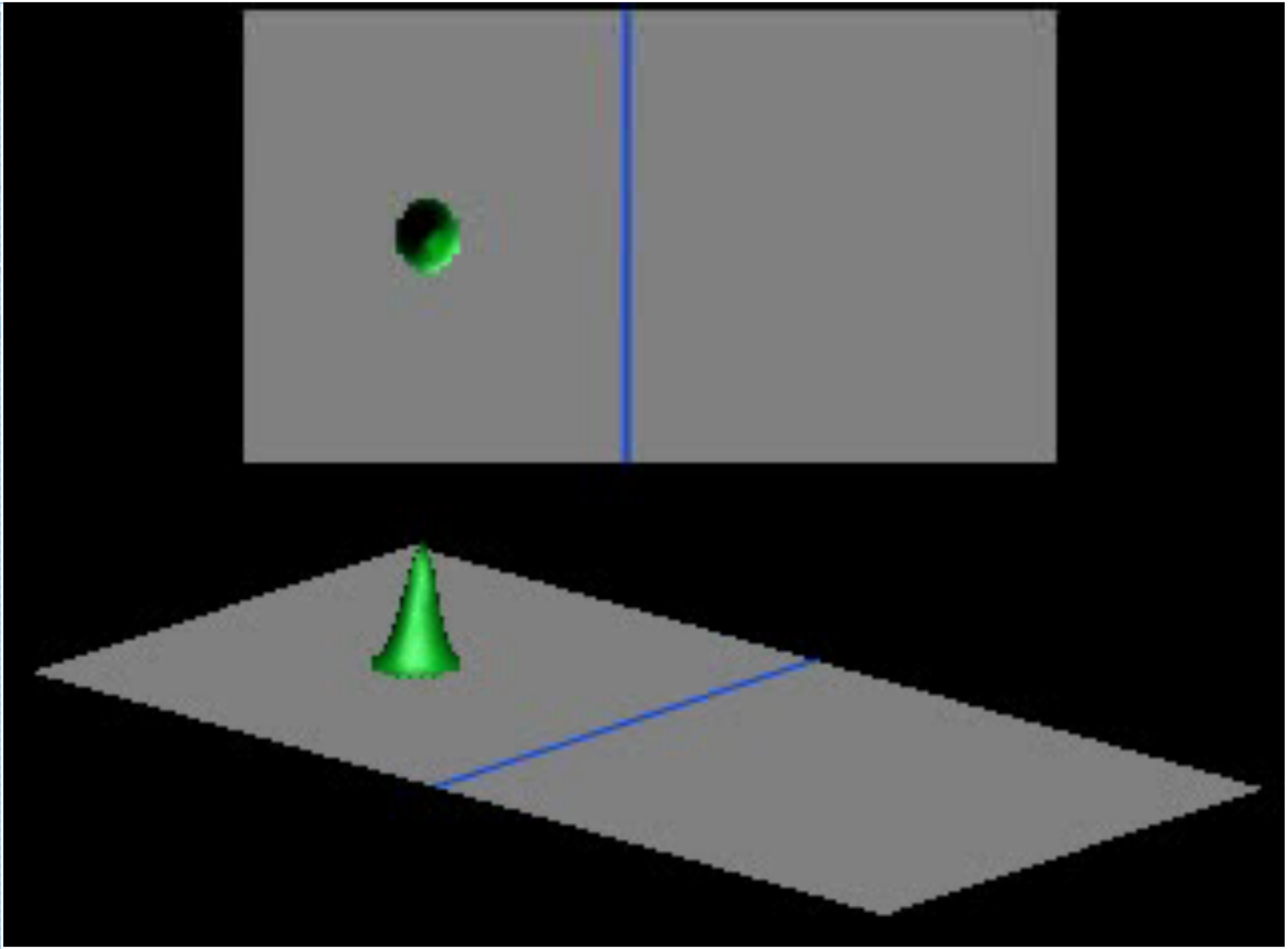
Charged particle in a constant magnetic field

To see this animations, visit: **http://www.embd.be/quantummechanics/**



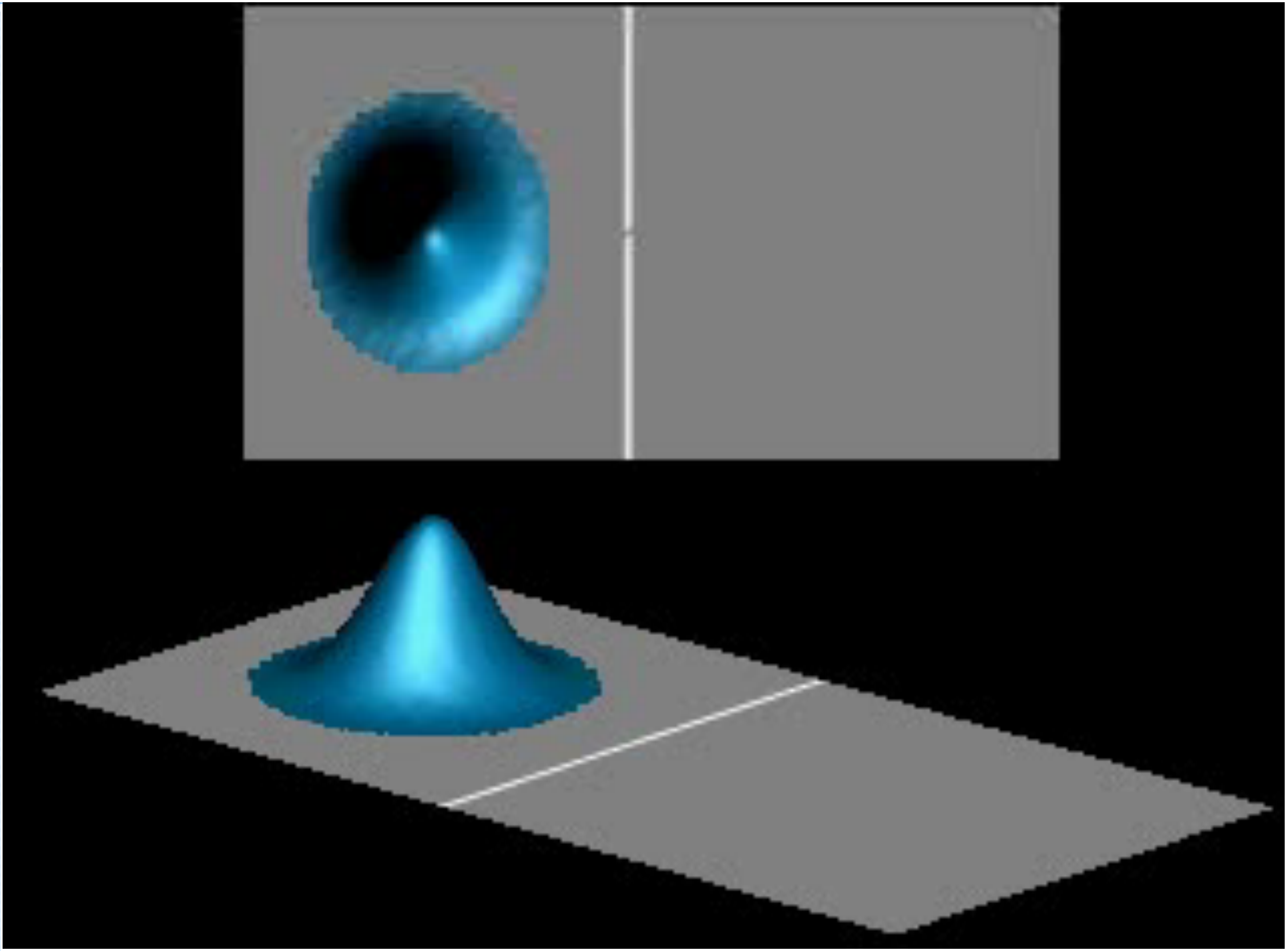
Charged particle in a constant magnetic field

To see this animations, visit: **http://www.embd.be/quantummechanics/**



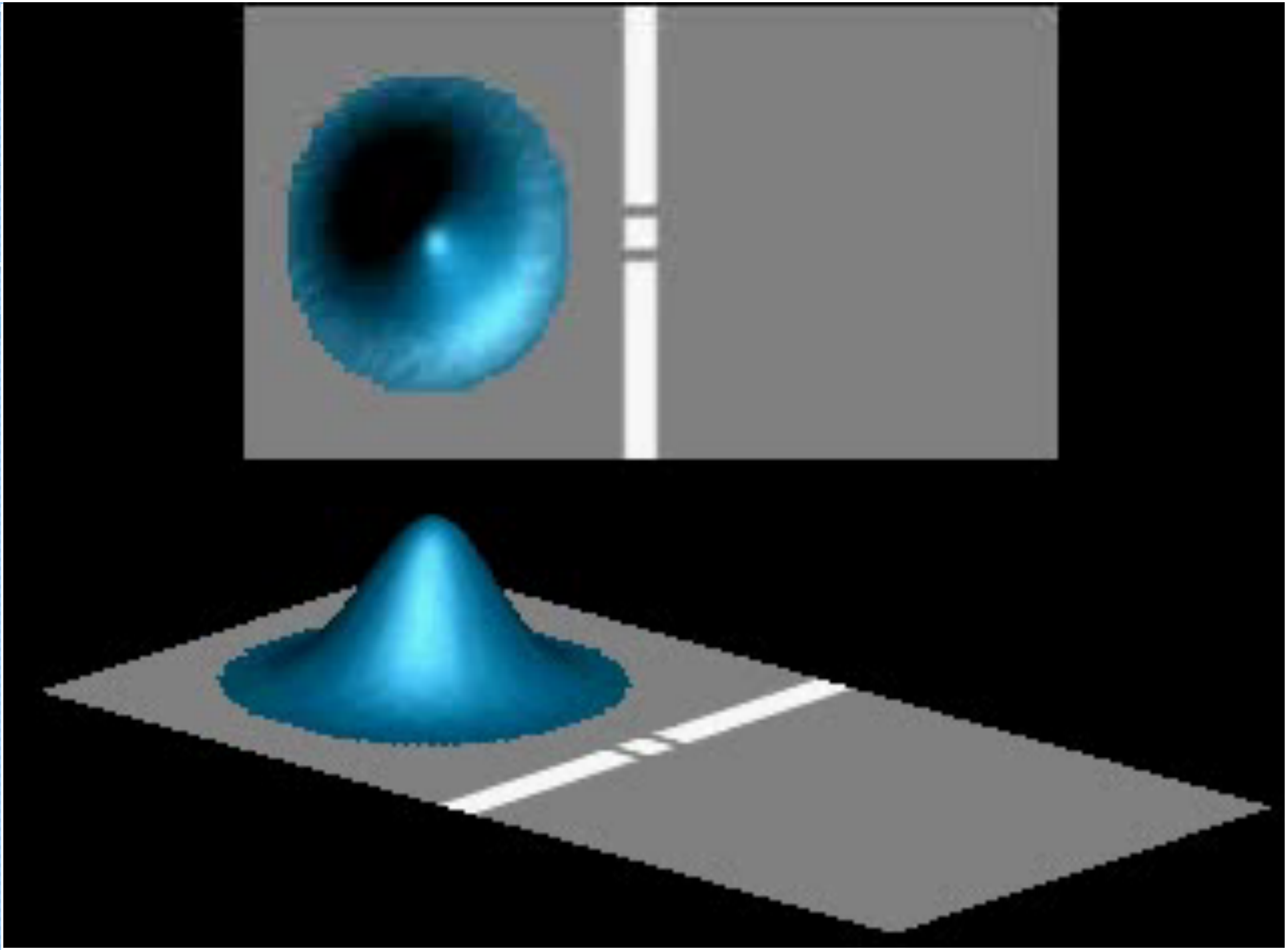
Tunnel effect

To see this animations, visit: **http://www.embd.be/quantummechanics/**



One slit diffraction

To see this animations, visit: **http://www.embd.be/quantummechanics/**



Two slits interference

To see this animations, visit: **http://www.embd.be/quantummechanics/**

Establishing possible levels of approximation

Strategies to approximate the scattering problem in theoretical methods

MODEL POTENTIAL
(one-particle wave functions) ➡

“ad-hoc” inclusion of
polarization effects

Simplifies the
Computational effort

MULTICHANNEL COUPLING
(many-body wave functions) ➡

Necessary to describe
electronic excitations,
Feshbach ressonances
and related processes

Skip it

Scattering theory

System Hamiltonian

$$H = H_N + T_{N+1} + V$$

H_N is the molecular target Hamiltonian with N electrons e M nuclei, *i.e.*,

$$H_N = \sum_{i=1}^{N} T_i + \sum_{i<j}^{N} \frac{1}{r_{ij}} - \sum_{\alpha,i}^{M,N} \frac{1}{r_{\alpha i}}$$

$$H_N \Phi_I = E_I \Phi_I$$

molecular problem is solved in a given level of approximation (Hartree-Fock, CI, etc.)

The projectile is a particle with T_{N+1} kinetic energy and interacts with the target through the scattering potential

$$V = -\sum_{A=1}^{M} \frac{Z_A}{\left|\vec{r}_{N+1} - \vec{R}_A\right|} + \sum_{j=1}^{N} \frac{1}{\left|\vec{r}_{N+1} - \vec{r}_j\right|}$$

Skip it

Scattering theory

Schrödinger equation

$$H\Psi_{\vec{k}_m}^{(\pm)}(\vec{r}_1,\cdots,\vec{r}_{N+1}) = E\Psi_{\vec{k}_m}^{(\pm)}(\vec{r}_1,\cdots,\vec{r}_{N+1})$$

Asymptotic condition

$$\Psi_{\vec{k}_i}^{(\pm)}(\vec{r}_1,\cdots,\vec{r}_{N+1}) \xrightarrow{r_{N+1}\to\infty} S_{\vec{k}_i} + \sum_{f}^{\text{open}} f^{B}_{i\to f}(\vec{k}_i,\vec{k}_f)\Phi_f \frac{e^{\pm i k_f r_{N+1}}}{r_{N+1}}$$

$$S_{\vec{k}_i} = \Phi_i e^{i\vec{k}_i\cdot\vec{r}_{N+1}}$$

Differential cross section

$$\frac{d\sigma^{i\to f}}{d\Omega}(\vec{k}_i,\vec{k}_f) = \frac{k_f}{k_i}\left|f^{L}_{i\to f}(\vec{k}_i,\vec{k}_f)\right|^2$$

Skip it

Scattering theory

Schrödinger differential equation

$$H\Psi_{\vec{k}_m}^{(\pm)} = \left[H_N + T_{N+1} + V\right]\Psi_{\vec{k}_m}^{(\pm)} = E\Psi_{\vec{k}_m}^{(\pm)}$$

Lippmann-Schwinger integral equation

$$\Psi_{\vec{k}_m}^{(\pm)} = S_{\vec{k}_m} + G_o^{(\pm)} V \Psi_{\vec{k}_m}^{(\pm)}$$

$$S_{\vec{k}_m} = \Phi_m e^{i\vec{k}_m \bullet \vec{r}_{N+1}}$$

Free-particle Green's function

$$G_o^{(\pm)} = \frac{1}{E - T_{N+1} - H_N \pm i\varepsilon} = \lim_{\varepsilon \to 0} \sum_m \int d^3k \, \frac{|\Phi_m \vec{k}\rangle\langle \vec{k}\Phi_m|}{\frac{k_m^2}{2} - \frac{k^2}{2} \pm i\varepsilon}$$

Skip it

Scattering theory

One-particle potential scattering

To obtain the scattering amplitude we write the Schrödinger integral equation in coordinate representation:

$$\Psi^{(+)}_{\vec{k}_i}(\vec{r}) = S_{\vec{k}_i}(\vec{r}) + \int G_0^{(+)}(\vec{r},\vec{r}\,')V(\vec{r}\,')\Psi^{(+)}_{\vec{k}_i}(\vec{r}\,')d\vec{r}\,'$$

A proper choice of poles for the Green's function gives:

$$\lim_{r\to\infty} \Psi^{(+)}_{\vec{k}_i}(\vec{r}) = S_{\vec{k}_i}(\vec{r}) - \frac{e^{+ikr}}{r}\frac{1}{4\pi}\int e^{-ik\hat{r}.\vec{r}\,'}V(\vec{r}\,')\Psi^{(+)}_{\vec{k}_i}(\vec{r}\,')d\vec{r}\,'$$

and furnishes the scattering amplitude as:

$$f(\theta,\phi) = -2\pi^2\int \frac{e^{-ik\hat{r}.\vec{r}\,'}}{(2\pi)^{3/2}}V(\vec{r}\,')\Psi^{(+)}_{\vec{k}_i}(\vec{r}\,')d\vec{r}\,'$$

Skip it

Schwinger Variational Principle

Using Dirac´s notation:

$$f_{\vec{k}_f,\vec{k}_i} = -2\pi^2 \langle \vec{k}_f \,|\, V \,|\, \Psi^{(+)}_{\vec{k}_i} \rangle$$

where $|\,\Psi^{(+)}_{\vec{k}_i}\rangle$ satisfies:

$$|\,\Psi^{(+)}_{\vec{k}_i}\rangle = |\,\vec{k}_i\rangle + G_0^{(+)} V \,|\, \Psi^{(+)}_{\vec{k}_i}\rangle$$

Multiplying this expression by V, we have:

$$V \,|\, \Psi^{(+)}_{\vec{k}_i}\rangle = V \,|\, \vec{k}_i\rangle + V G_0^{(+)} V \,|\, \Psi^{(+)}_{\vec{k}_i}\rangle$$

$$\boxed{A^{(+)} \,|\, \Psi^{(+)}_{\vec{k}_i}\rangle = V \,|\, \vec{k}_i\rangle}$$

where: $$A^{(+)} = V - V G_0^{(+)} V$$

Skip it

Schwinger Variational Principle

It is also possible to write Lippmann-Schwinger equation for:

$$|\Psi^{(-)}_{\vec{k}_f}\rangle = |\vec{k}_f\rangle + G_0^{(-)} V |\Psi^{(-)}_{\vec{k}_f}\rangle$$

with:

$$G_0^{(-)}(\vec{r},\vec{r}\,') = -\frac{1}{4\pi}\frac{e^{-ik|\vec{r}-\vec{r}\,'|}}{|\vec{r}-\vec{r}\,'|}$$

For this boundary condition, we have

$$\boxed{A^{(-)}|\Psi^{(-)}_{\vec{k}_f}\rangle = V|\vec{k}_f\rangle}$$

where:

$$A^{(-)} = V - VG_0^{(-)}V$$

$$f_{\vec{k}_f,\vec{k}_i} = -2\pi^2\langle\Psi^{(-)}_{\vec{k}_f}|V|\vec{k}_i\rangle$$

Skip it

Schwinger Variational Principle

So, our problem is to solve the equations:

$$\boxed{A^{(\pm)}|\Psi^{(\pm)}_{\vec{k}_m}\rangle = V|\vec{k}_m\rangle}$$

and with the solutions to get the scattering amplitudes

$$f_{\vec{k}_f,\vec{k}_i} = -2\pi^2\langle\vec{k}_f|V|\Psi^{(+)}_{\vec{k}_i}\rangle = -2\pi^2\langle\Psi^{(-)}_{\vec{k}_f}|V|\vec{k}_i\rangle$$

The Schwinger variational expression for the amplitude is given by:

$$[f_{\vec{k}_f,\vec{k}_i}] = -2\pi^2\{\langle\vec{k}_f|V|\Psi^{(+)}_{\vec{k}_i}\rangle + \langle\Psi^{(-)}_{\vec{k}_f}|V|\vec{k}_i\rangle$$
$$-\langle\Psi^{(-)}_{\vec{k}_f}|A^{(+)}|\Psi^{(+)}_{\vec{k}_i}\rangle\}$$

Skip it

Schwinger Variational Principle

$$[\delta f_{\vec{k}_f,\vec{k}_i}] = 0 \rightarrow A^{(\pm)}\,|\Psi^{(\pm)}_{\vec{k}_m}\rangle = V\,|\vec{k}_m\rangle$$

Expansion of the scattering wave functions in a trial basis $\{\chi_\mu\}$:

$$|\Psi^{(\pm)}_{\vec{k}_m}\rangle = \sum_{\mu} a^{(\pm)}_{\mu}(\vec{k}_m)\,|\chi_\mu\rangle$$

and the application of the variational principle over the expansion coefficients

$$\frac{\partial[f_{\vec{k}_f,\vec{k}_i}]}{\partial a^{(\pm)}_{\mu}} = 0 \rightarrow f_{\vec{k}_i,\vec{k}_f} = -2\pi^2 \sum_{mn} \langle \vec{k}_f|V|\chi_m\rangle (d^{-1})_{mn} \langle \chi_n|V|\vec{k}_i\rangle$$

where $d_{mn} = \langle \chi_m|A^{(+)}|\chi_n\rangle$ and $A^{(+)} = V - VG_0^{(+)}V$

Skip it

Schwinger Variational Principle

MAIN ADVANTAGES

❶ Boundary conditions are introduced through the Green's function $G_0^{(+)}$

❷ Expansion of the scattering wave function can be done in a basis of square integrable functions (Cartesian Gaussian functions)

IMPORTANT REQUIREMENT

❸ The VGV terms must be evaluated numerically, through a linear momentum quadrature scheme

MAIN DRAWBACK

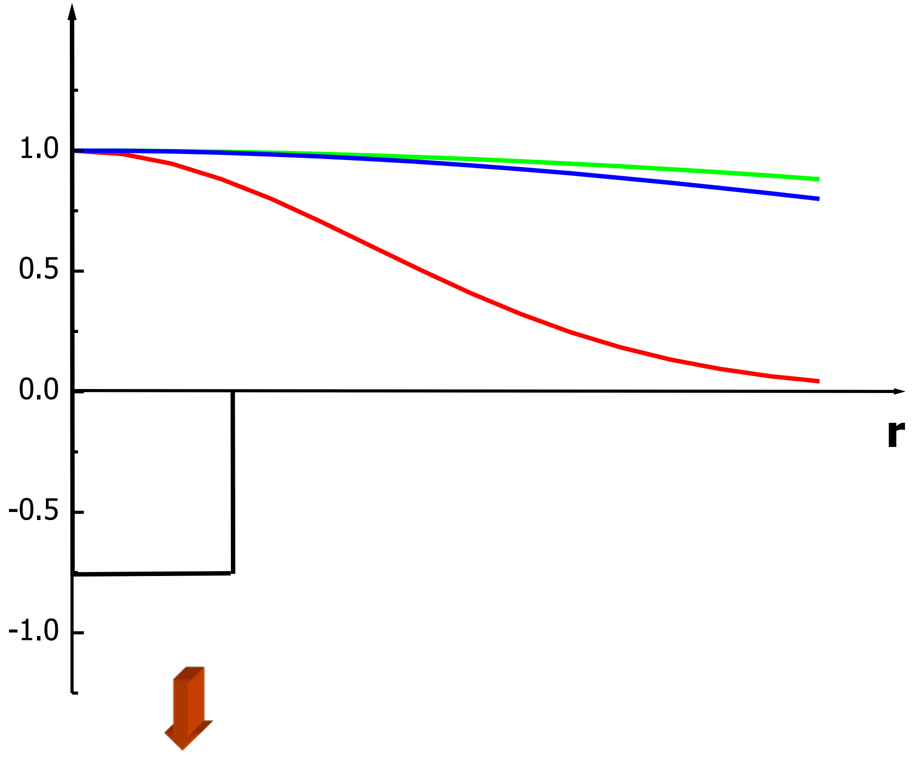
❹ Susceptible to numerical problems

Skip it

Origin of the numerical instability

SHORT RANGE POTENTIALS AND FUNCTIONS TOO DIFUSE CAN GENERATE LINEAR DEPENDENCY IN THE TRIAL BASIS $\{|\chi_\mu\rangle\}$

Typical Situation:



gives rise to spurious structures of numerical nature

Skip it

Schwinger Multichannel Method for electron scattering

In this formalism the operator $A^{(+)}$ was redefined as:

$$A^{(+)} = \frac{1}{2}(PV + VP) - VG_P^{(+)}V + \frac{1}{N+1}\left[\hat{H} - \frac{N+1}{2}(\hat{H}P + P\hat{H})\right]$$

where $P \equiv \sum_{\ell=1}^{\text{open}} |\Phi_\ell\rangle\langle\Phi_\ell|$ and $\hat{H} = E - H$

All electrons are identical. So, an expansion of the scattering wave function must be done in a basis $\{\chi_\mu\}$ of anti-symmetric functions (Slater determinants):

$$|\Psi_{\vec{k}_m}^{(\pm)}\rangle = \sum_\mu a_\mu^{(\pm)}(\vec{k}_m)\,|\chi_\mu\rangle \quad \text{where} \quad \{|\chi_\mu\rangle\} = \{a_{N+1}\,|\Phi_i\rangle \otimes |\varphi_j\rangle\}$$

The final form of the scattering amplitude is equal to the one of the Schwinger Variational principle

$$f_{\vec{k}_i,\vec{k}_f} = -\frac{1}{2\pi}\sum_{mn}\langle S_{\vec{k}_f}|V|\chi_m\rangle(d^{-1})_{mn}\langle\chi_n|V|S_{\vec{k}_i}\rangle$$

with $d_{mn} = \langle\chi_m|A^{(+)}|\chi_n\rangle$ and $S_{\vec{K}_i} \equiv \Phi_i(\vec{r}_1,\ldots,\vec{r}_N)\, e^{i\vec{K}_i\cdot\vec{r}_{N+1}}$

Skip it

K. Takatsuka and V. McKoy, Phys. Rev. A **24**, 2473 (1981)

Instituto de Física Gleb Wataghin
UNICAMP

R. F. da Costa, F. J. da Paixão and M.A. P. Lima,
J. Phys. B **38**, 4363 (2005)

Coupling level

Elastic scattering with and without polarization effects

❶ Open channel Projector has only one state

$$P = |\Phi_o\rangle\langle\Phi_o|$$

Φ_o is molecular target ground state obtained in Hartree-Fock approximation

❷ Configuration space is made of

$$|\chi_\mu\rangle = \begin{cases} a_{N+1}\,|\Phi_o\rangle \otimes |\varphi_i\rangle \\ a_{N+1}\,|\Phi_j\rangle \otimes |\varphi_k\rangle, j \geq 2 \end{cases}$$

Doublet states made of products of target triplet and singlet states by φ_k

Φ_j , j ≥ 2 are virtual states obtained from single excitations of the molecular target

φ_i are one-particle wave functions (square integrable molecular orbitals) used in description of the continuum

Skip it

R. F. da Costa, F. J. da Paixão and M.A. P. Lima,
J. Phys. B **38**, 4363 (2005)

Coupling level

Inelastic scattering with and without polarization

❶ Open channel projector contains channels of our choice (truncation means approximation)

$$P = \sum_{\ell}^{\text{open}} |\Phi_\ell\rangle\langle\Phi_\ell|$$

$|\Phi_\ell\rangle$ are molecular target states obtained with single configuration interaction

❷ Again the configuration space is made of

$$|\chi_\mu\rangle = \begin{cases} a_{N+1}|\Phi_o\rangle\otimes|\varphi_i\rangle \\ a_{N+1}|\Phi_j\rangle\otimes|\varphi_k\rangle, j \geq 2 \end{cases}$$

Doublet states made of products of target triplet and singlet states by φ_k

Polarization effects are included with j greater than the number of open channels

Skip it

Electron scattering by large molecules

Pseudopotential formalism

[D. R. Hamann, M. Schlüter and C. Chiang, Phys. Rev. Lett. **43**, 1494 (1979)]

❶ The pseudo-state energy is equal to the real eigenvalue for a given configuration;

❷ The pseudopotential is equal to the real potential beyond a certain core radius r_c, and it is soft at the origin;

❸ The normalized pseudo wave function is equal to the real one beyond the core radius r_c and it is soft and without nodes

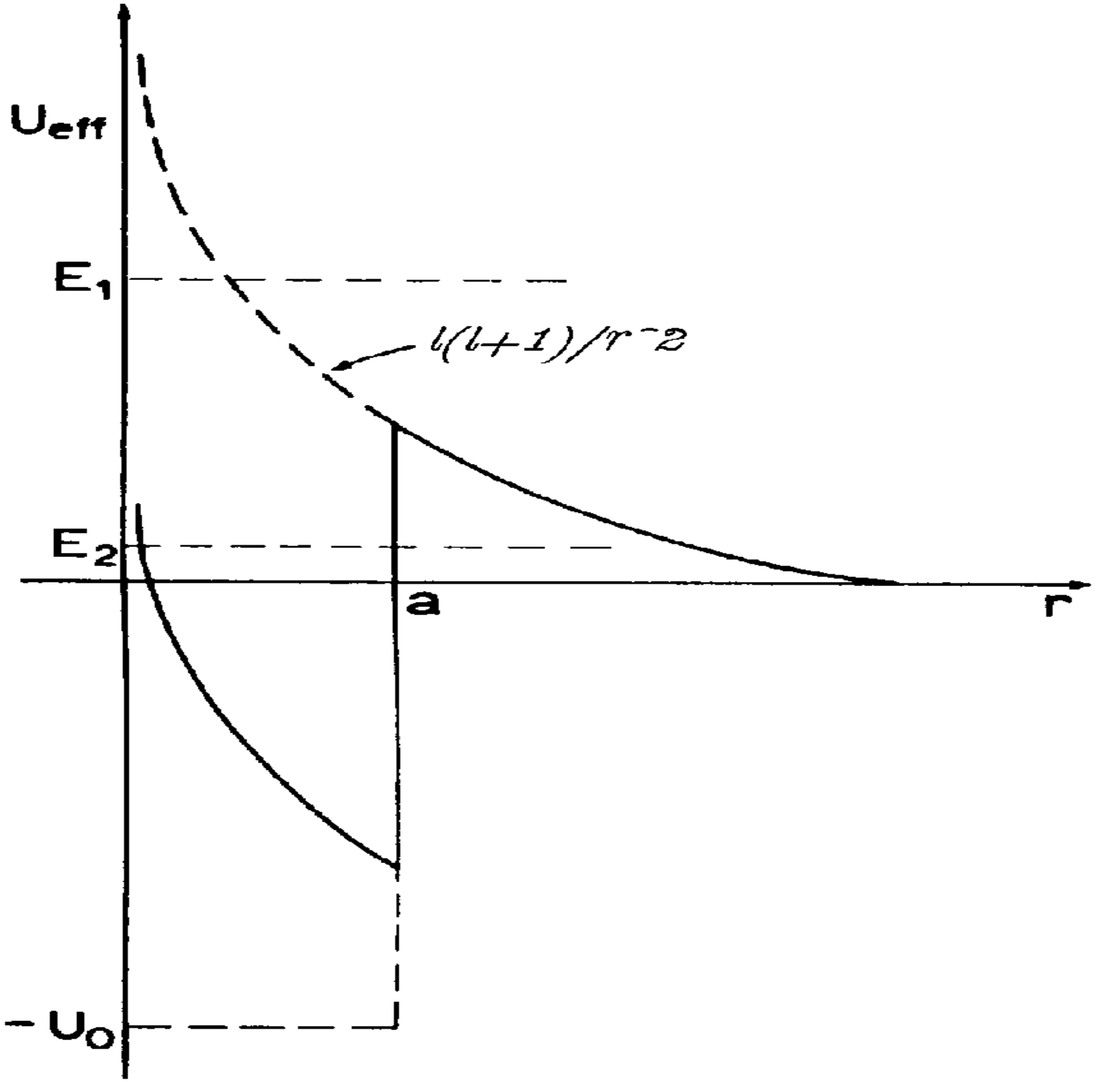
❹ The integrals from 0 to r of the real and pseudo functions agree for $r > r_c$ for each valence state:

$$-\frac{1}{2}\left[(r\Psi)^2\frac{d}{dE}\frac{d}{dr}\ln\Psi\right]_{r>r_c} = \int_0^{r>r_c}\Psi^2 r^2 dr$$

"Norm Conservation"

Skip it

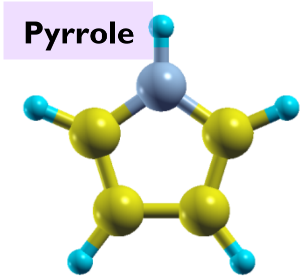
Shape resonances are related to angular momentum traps

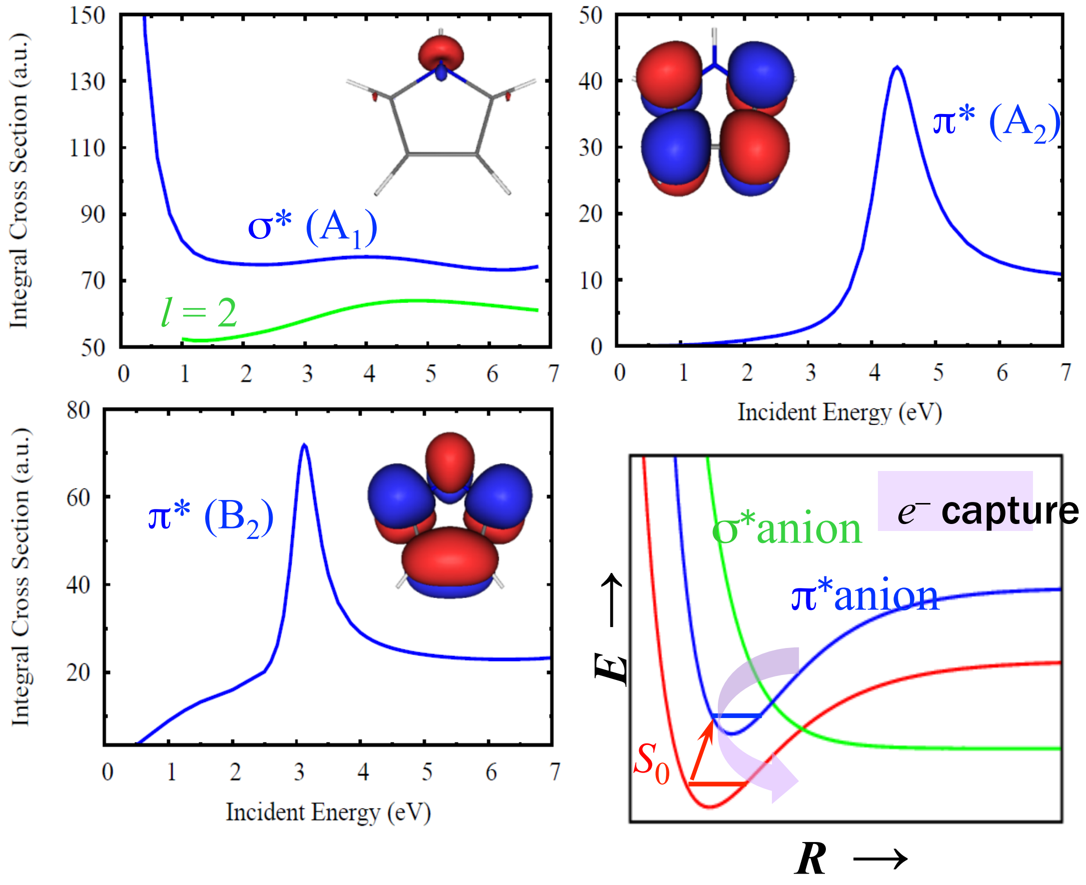


Back to it

Low energy elastic electron scattering from pirrole

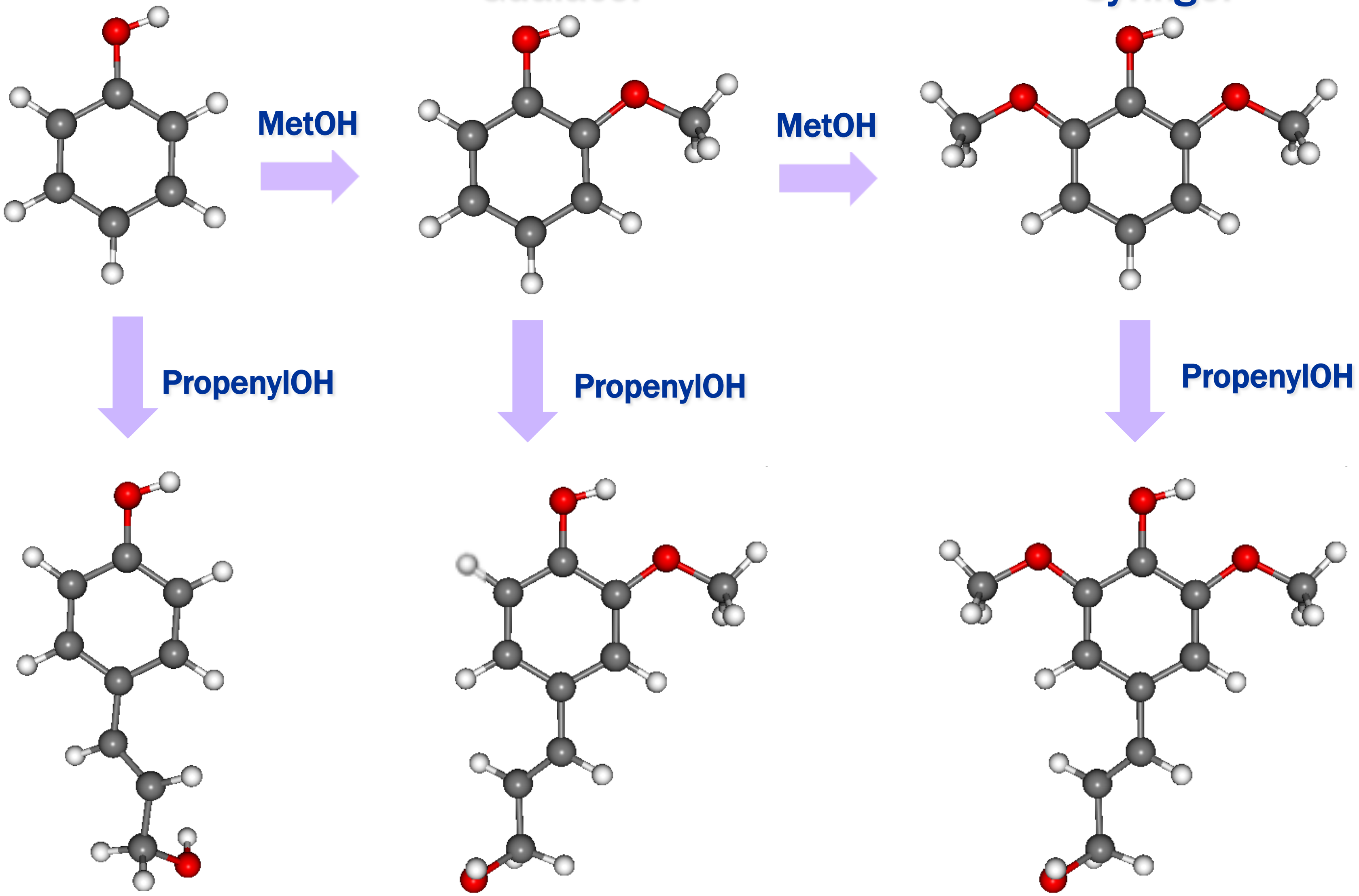
- There are π^* (ring) and σ^* (N–H) shape resonances in pyrrole. Nice prototype!





de Oliveira EM, Lima MAP, Bettega MHF, Sanchez SD, da Costa RF, and Varella MTD, J. Chem. Phys. **132**, 204301 (2010)

Lignin Subunits



Phenol → MetOH → **Guaiacol** → MetOH → **Syringol**

PropenylOH

PropenylOH

PropenylOH

***p*-coumaryl alcohol**

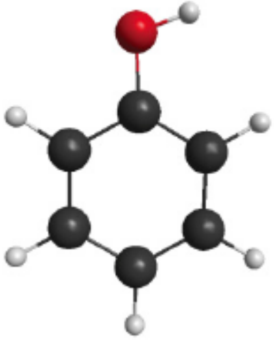
coniferyl alcohol

sinapyl alcohol

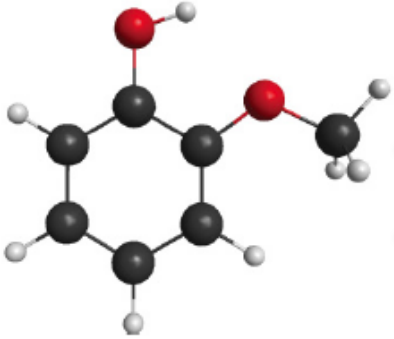
RAPID COMMUNICATIONS

Shape resonance spectra of lignin subunits

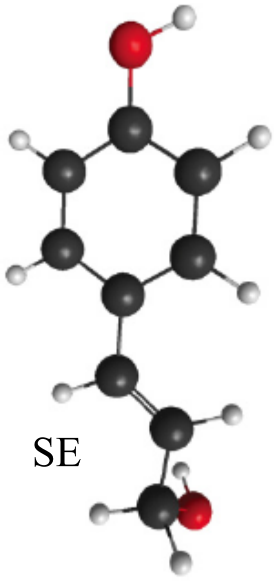
PHYSICAL REVIEW A **86**, 020701(R) (2012)



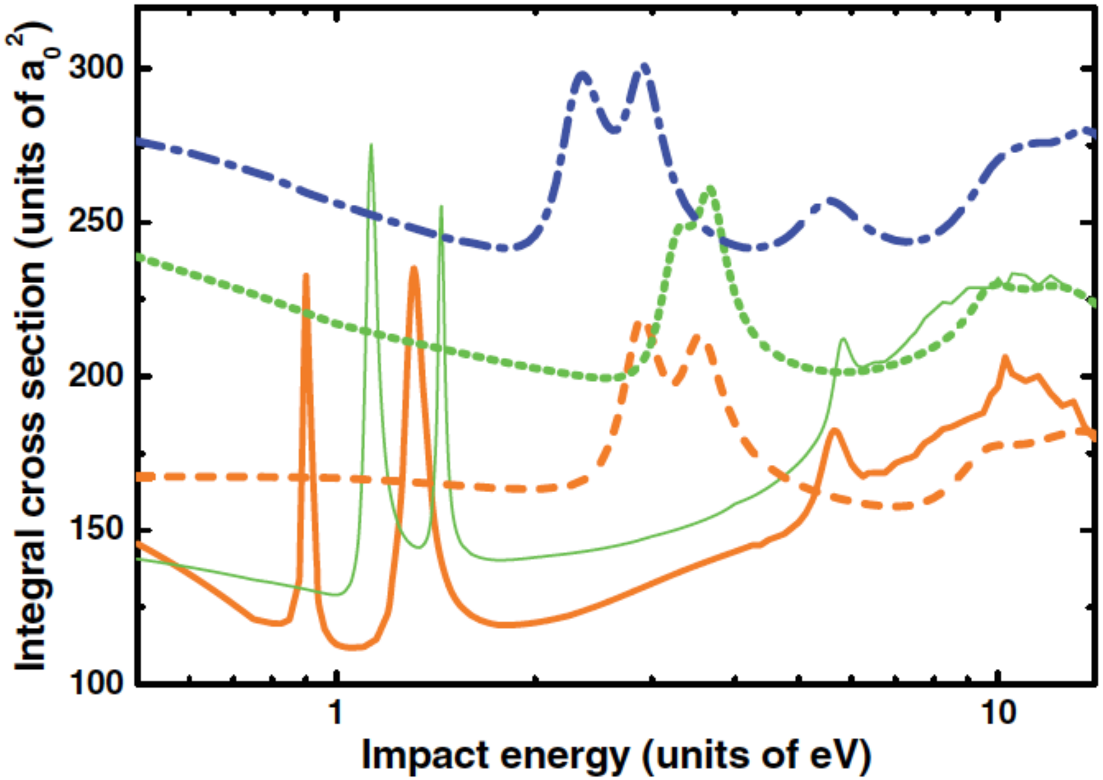
phenol



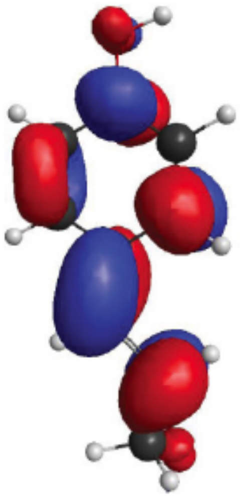
guaiacol

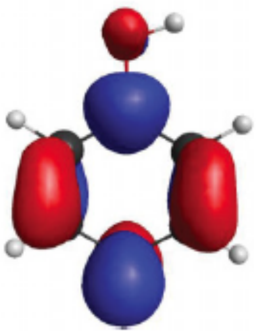


***p*-coumaryl alcohol**

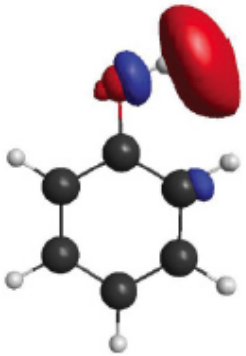


p-Cu (LUMO)



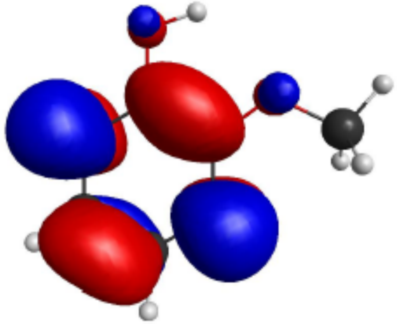


π* (LUMO+1)

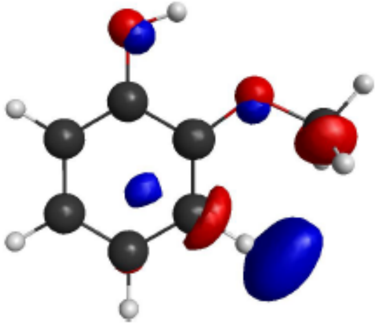


σ* (LUMO+2)

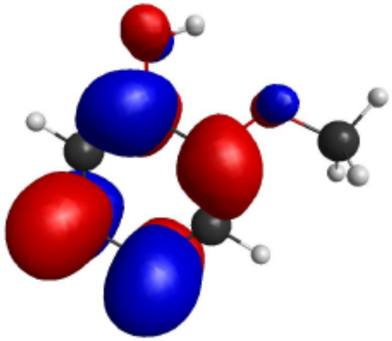
Phenol: Calculations, ET spectra and DEA data indicate H elimination from π*/σ* coupling.



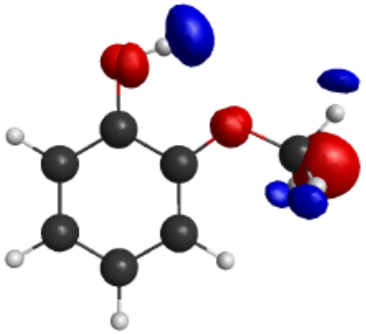
π* (LUMO)



σ* (LUMO+2)



π* (LUMO+1)

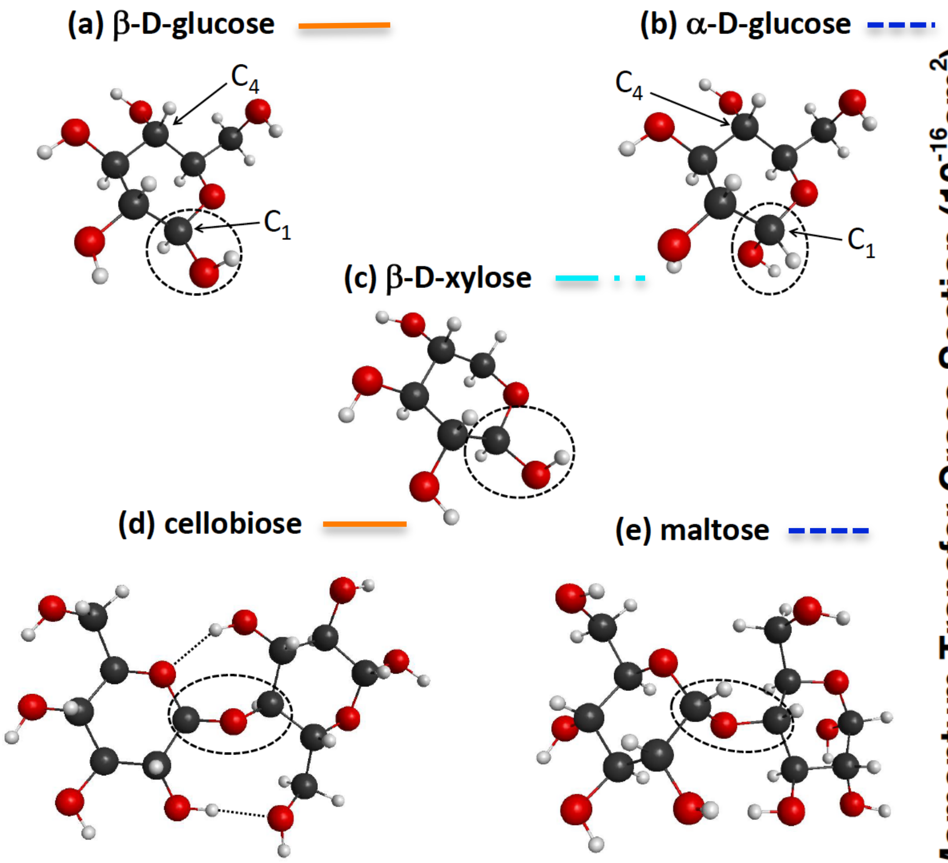


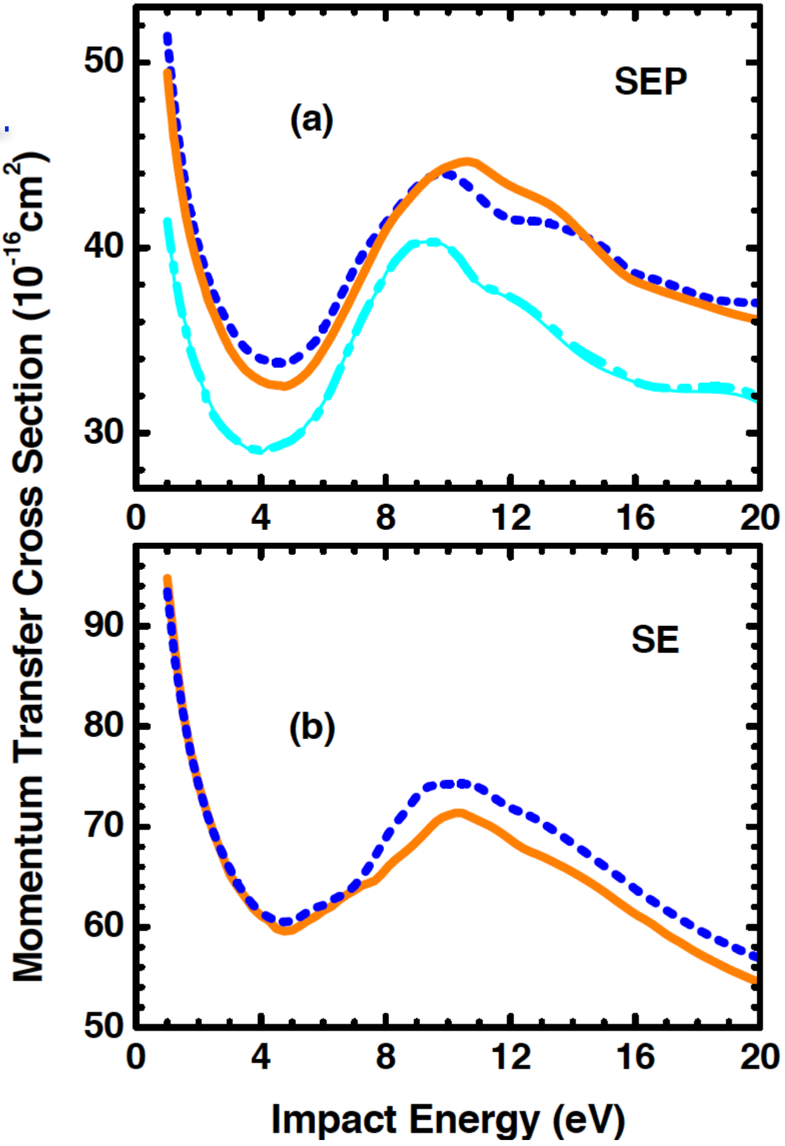
σ* (LUMO+3)

Guaiacol: Methoxilation is expected to give rise to other dissociation channels. H elimination should be also observed.

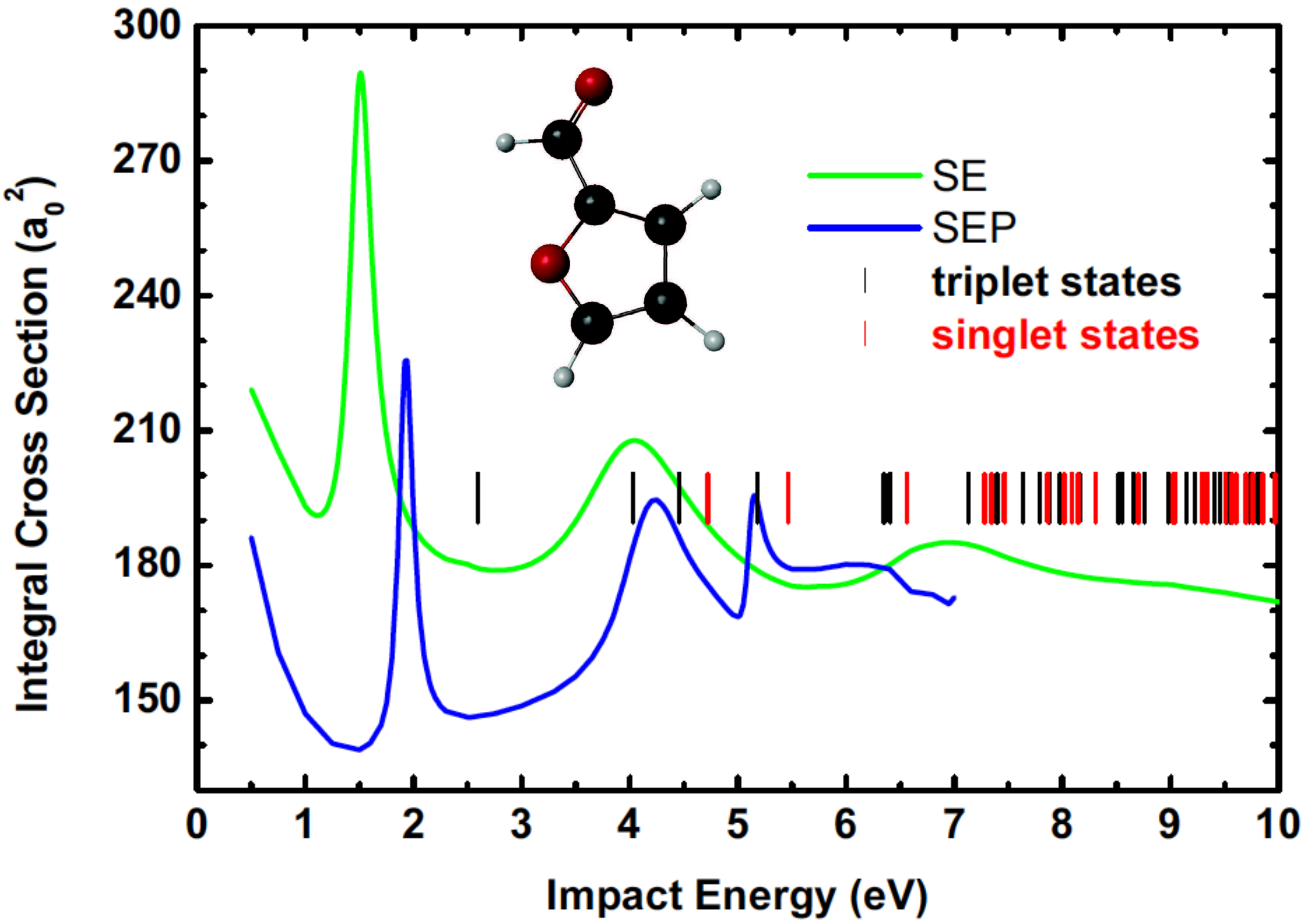
Low-energy electron scattering by cellulose and Hemicellulose components

Phys. Chem. Chem. Phys. **15**, 1682 (2013).





Electron Scattering of slow electrons by furfural molecules



This molecule has over 50 electronic states between 0 and 10 eV

Theoretical team on electron-scattering of microsolvated molecules

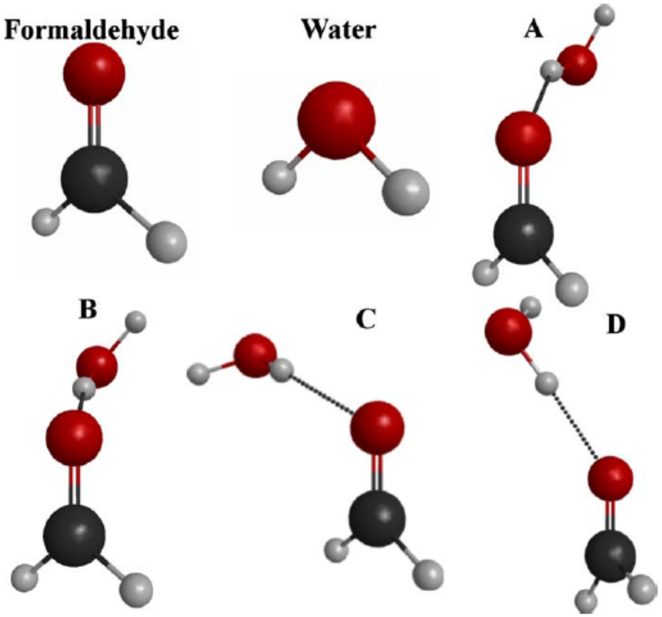
Sylvio Canuto (microsolvation)
Kaline Coutinho (microsolvation)
Márcio T. do N. Varella

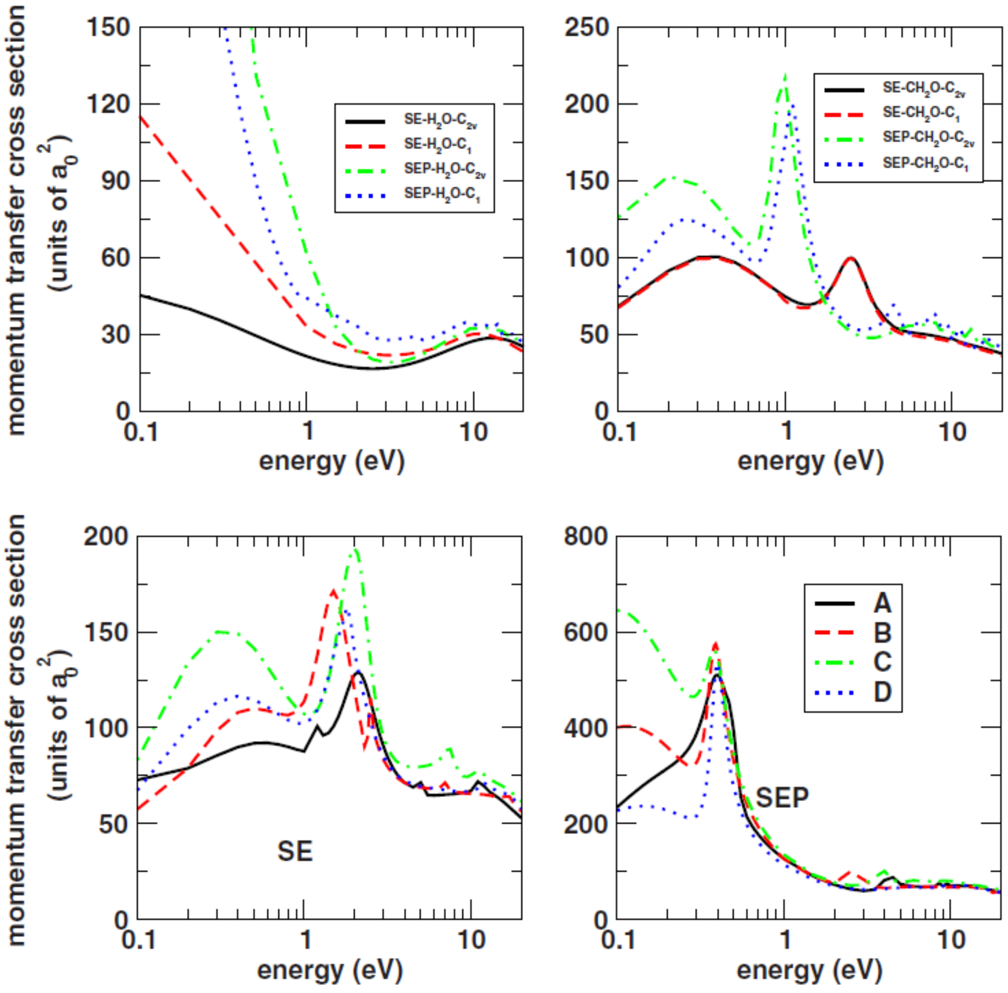
Eliane M. de Oliveira (scattering of solvated phenol)
Marco A. P. Lima

Thiago C. Freitas (his Ph.D. Thesis)
Márcio H. F. Bettega (coordinator)

Electron Collisions with the CH_2O-H_2O complex

PHYSICAL REVIEW A 80, 062710 (2009)





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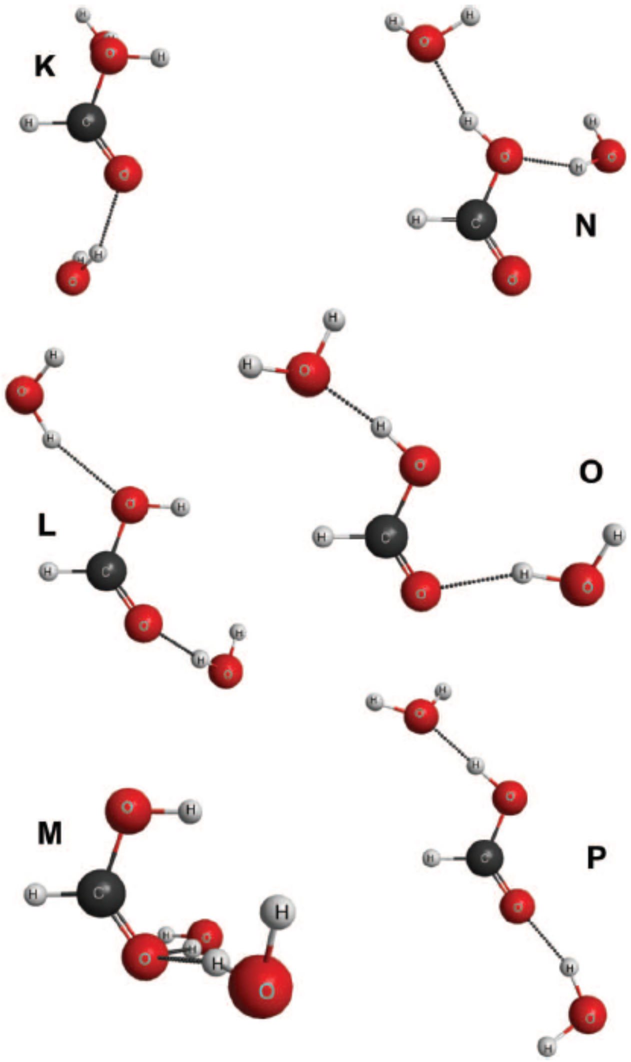
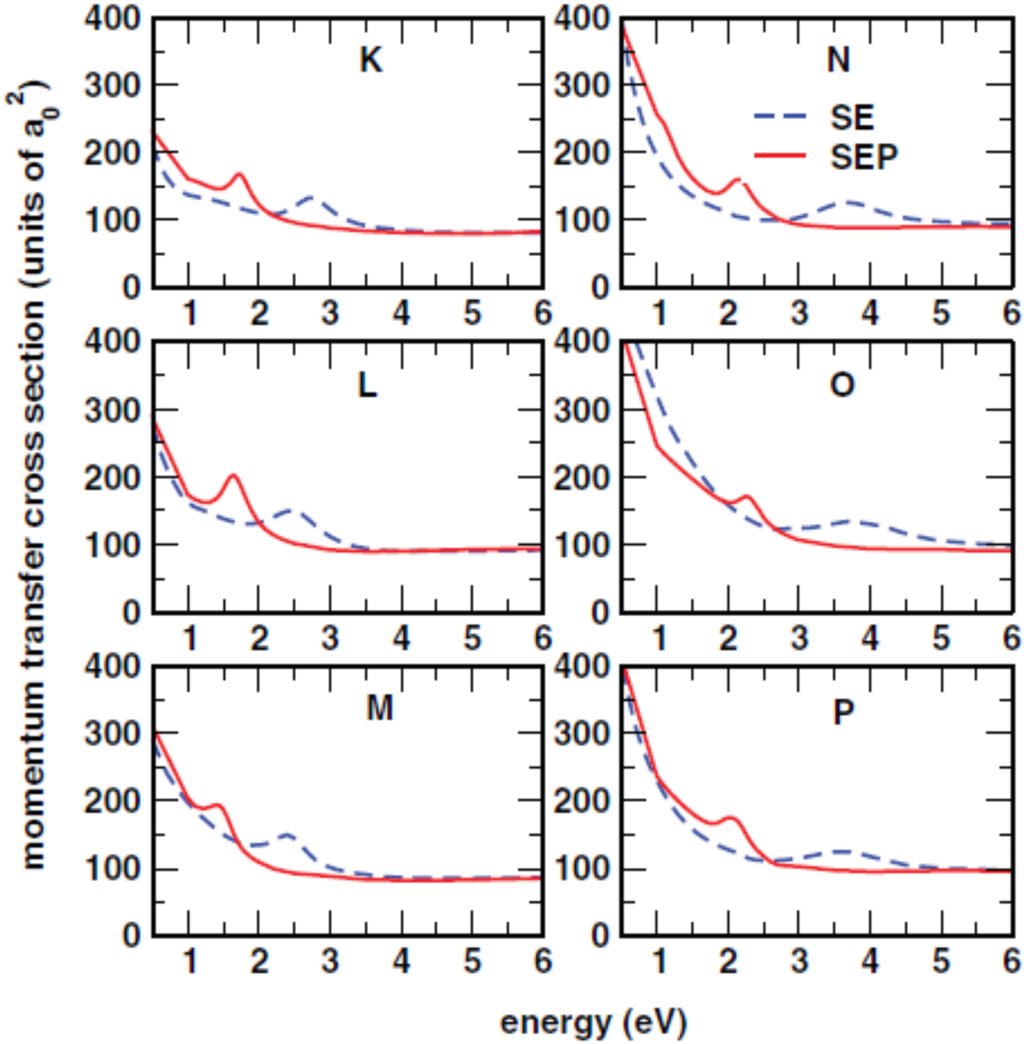
Electron collisions with the HCOOH…(H_2O)n complexes (n=1, 2) in liquid phase: The influence of microsolvation on the π^* resonance of formic acid

THE JOURNAL OF CHEMICAL PHYSICS **138**, 174307 (2013)

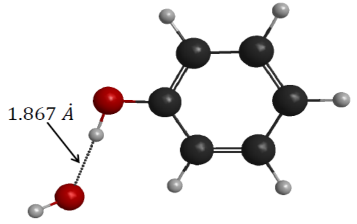


π^* shape resonance for HCOOH at around 1.9 eV.

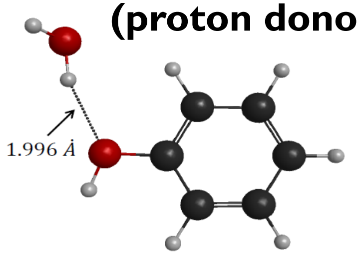


Electron Collisions with Phenol...H_2O

(proton acceptor)

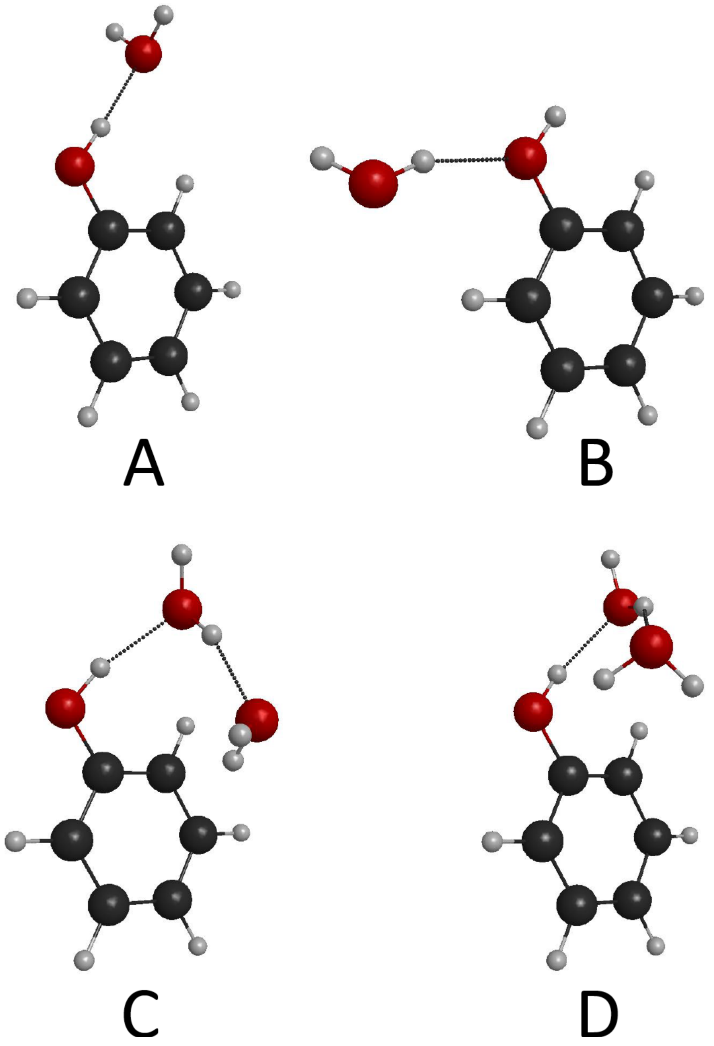


(proton donor)



We have studied the microsolvation of Phenol using 4 complexes.

- In Complex A, the water molecule is a proton acceptor.
- In the Complex B, the water is a proton donor.
- Complexes C and D have both situations (one water molecule as acceptor and the other as proton donor).



Electron Collisions with Phenol...H_2O

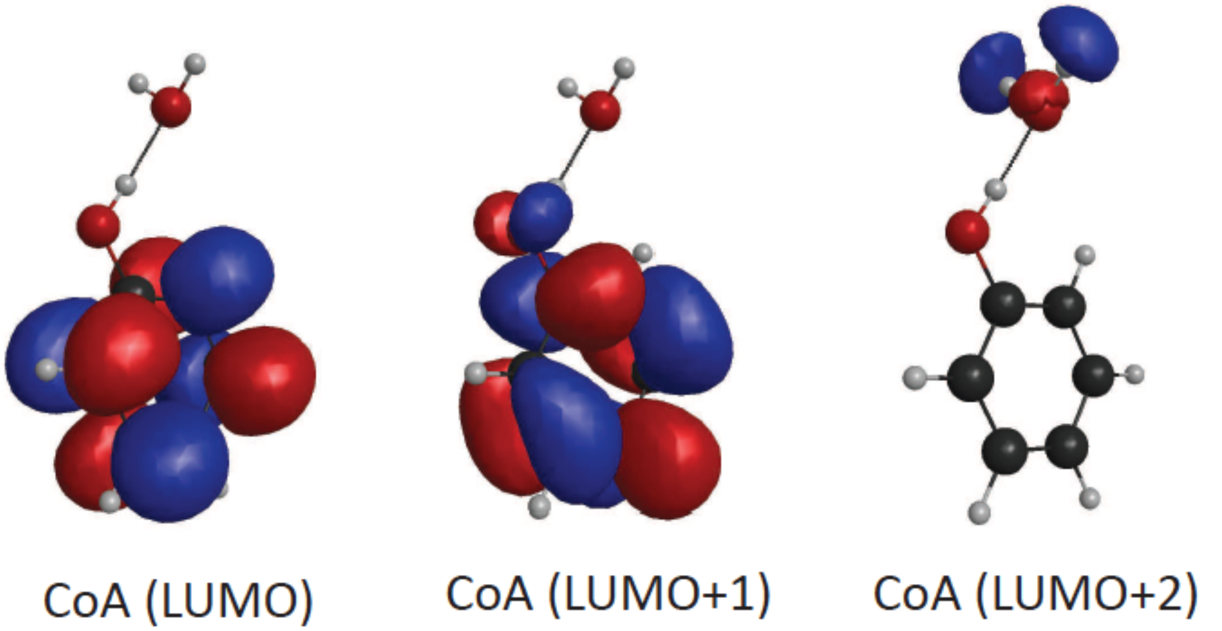


FIG. 1. (Color online) The three lowest virtual orbitals of the complex *A*.

Electron Collisions with Phenol...H_2O

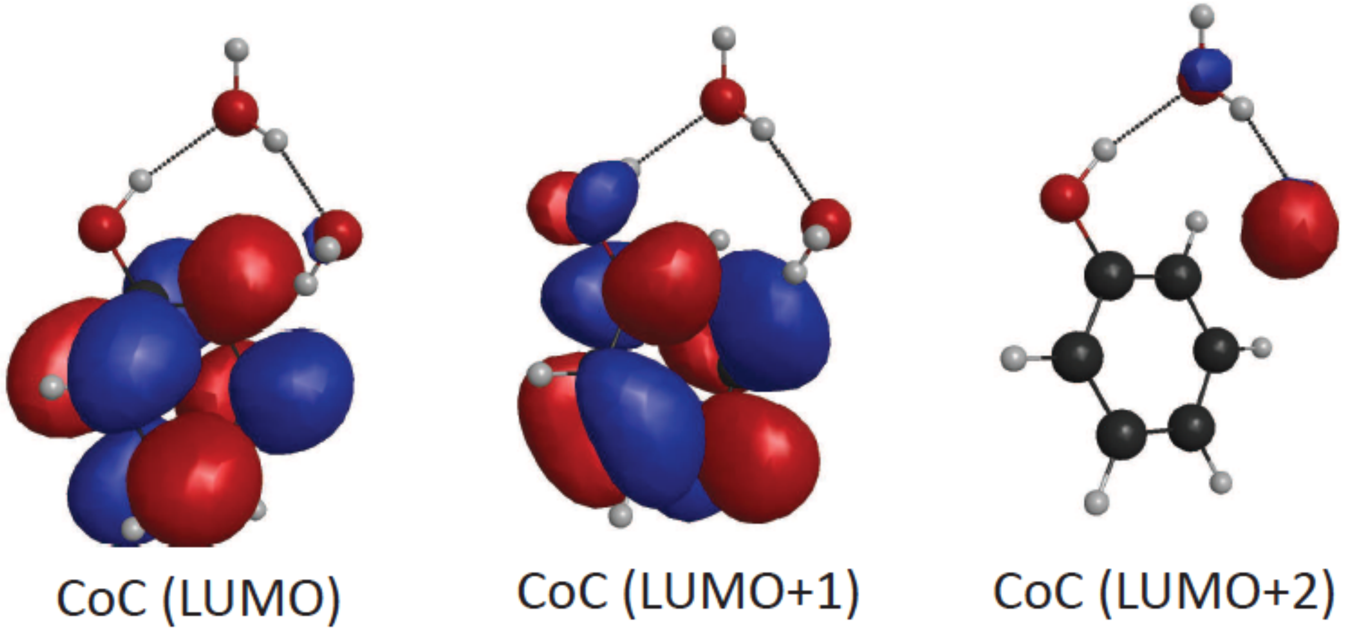
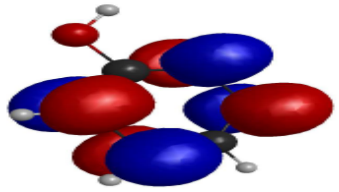


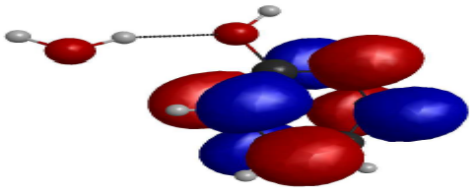
FIG. 2. (Color online) Same as in Fig. 1, but for the complex C.

Electron Collisions with Phenol...H_2O

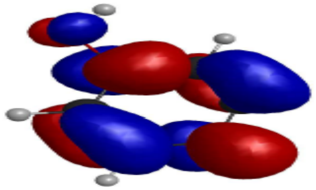
Ph (LUMO)



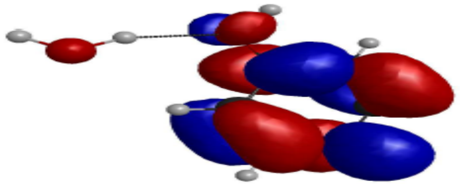
CoB (LUMO)



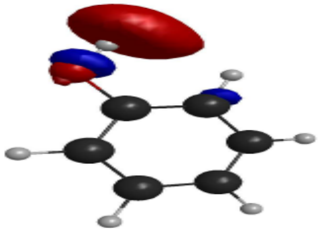
Ph (LUMO+1)



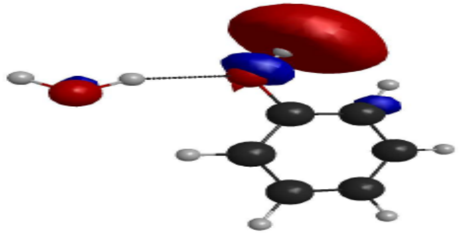
CoB (LUMO+1)



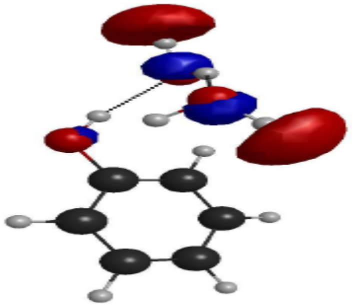
Ph (LUMO+2)



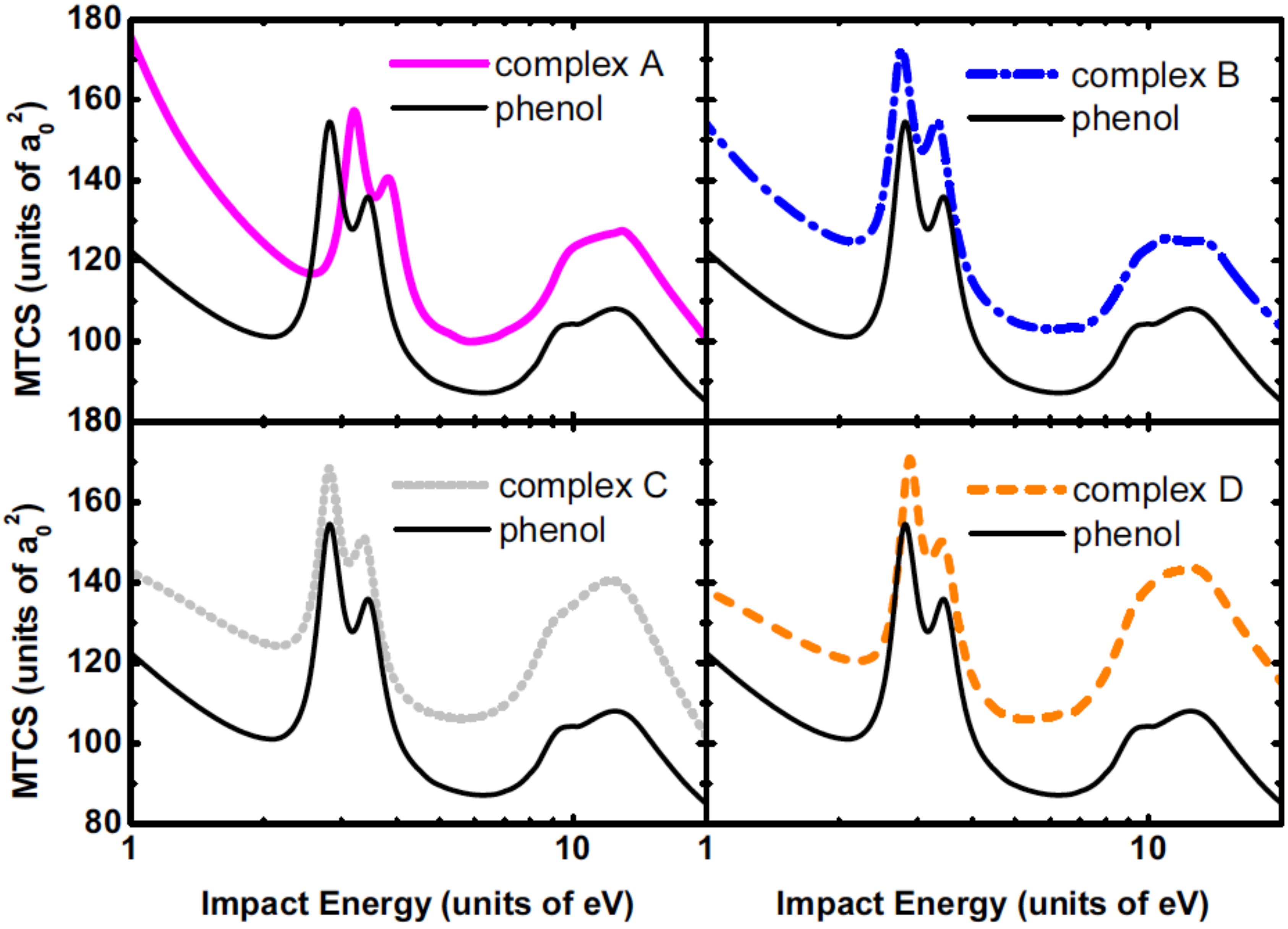
CoB (LUMO+2)



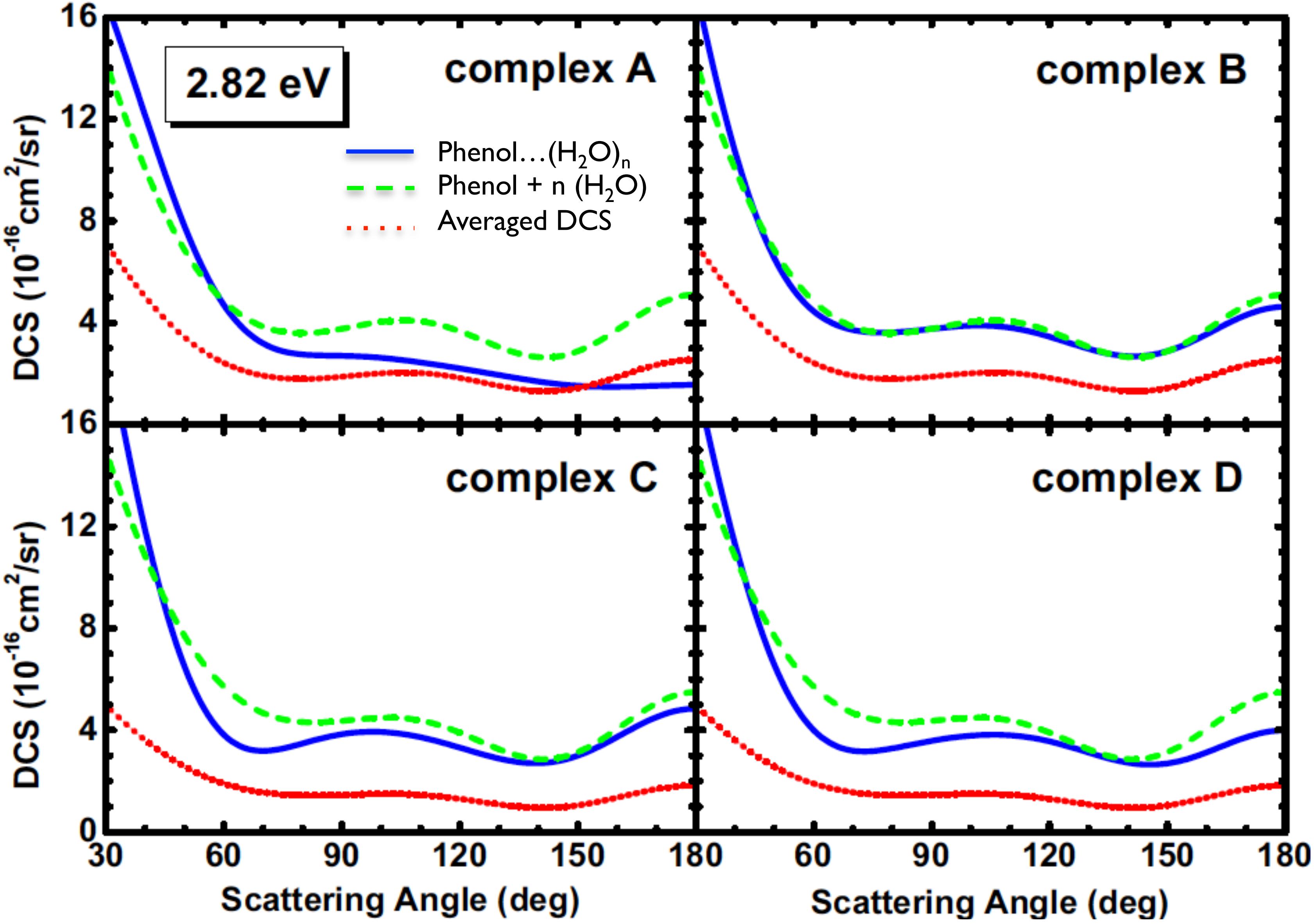
CoD (LUMO+2)



Electron Collisions with Phenol...$(H_2O)_n$: n=1,2

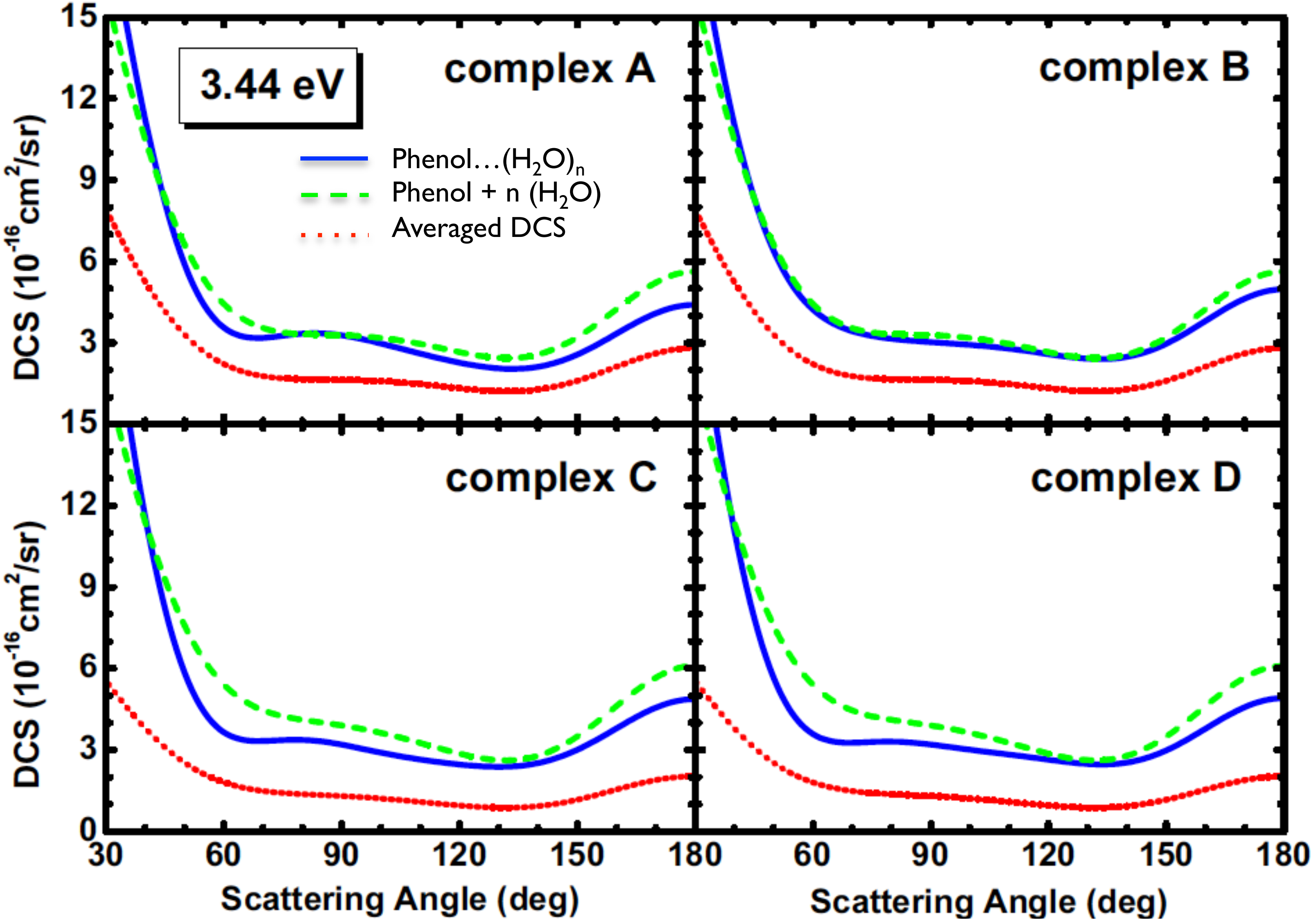


Electron Collisions with Phenol...$(H_2O)_n$: search for microsolvation signatures in the DCS



IFT
ICTP-SAIFR
2014
São Paulo

Electron Collisions with Phenol...$(H_2O)_n$: search for microsolvation signatures in the DCS



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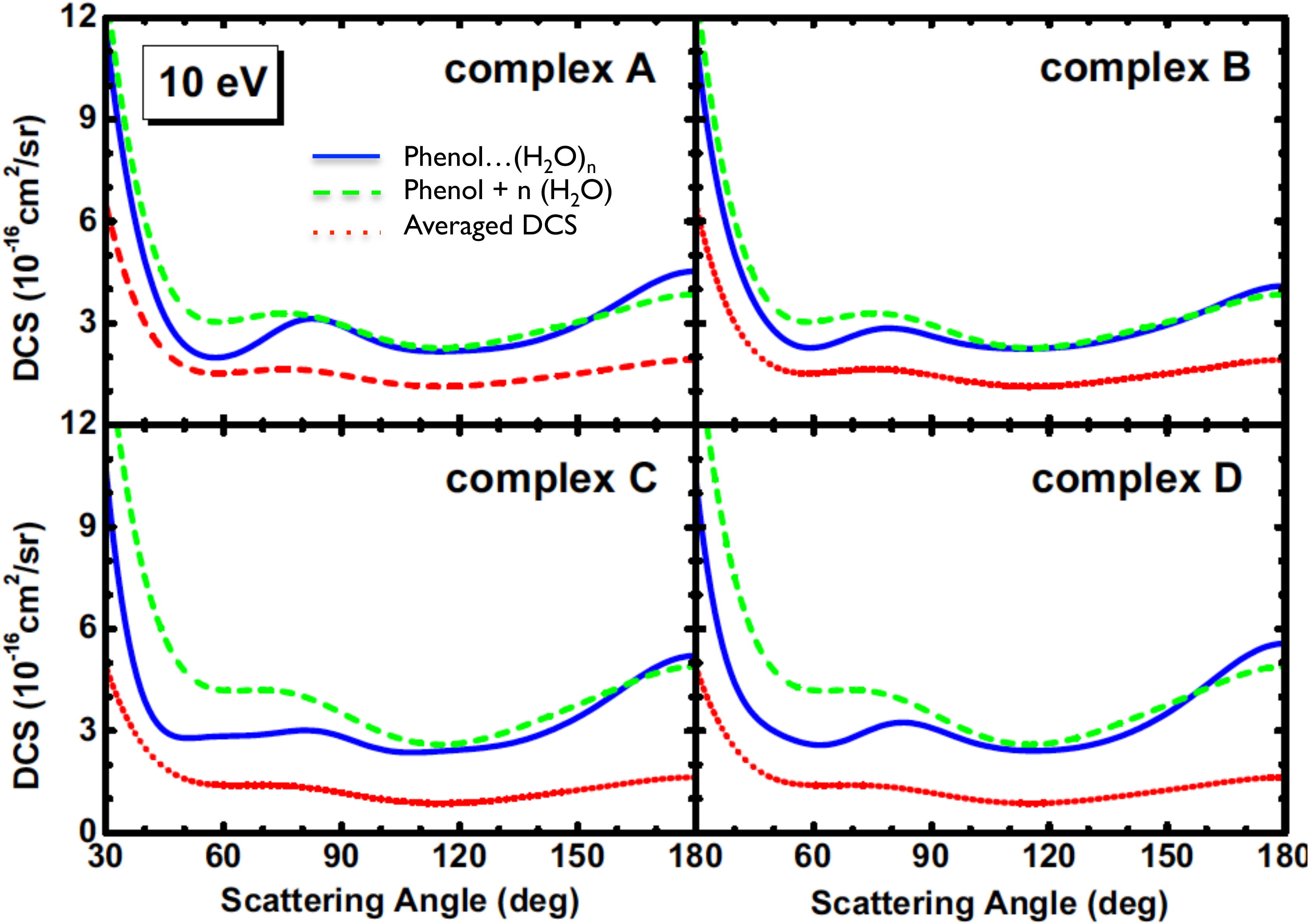
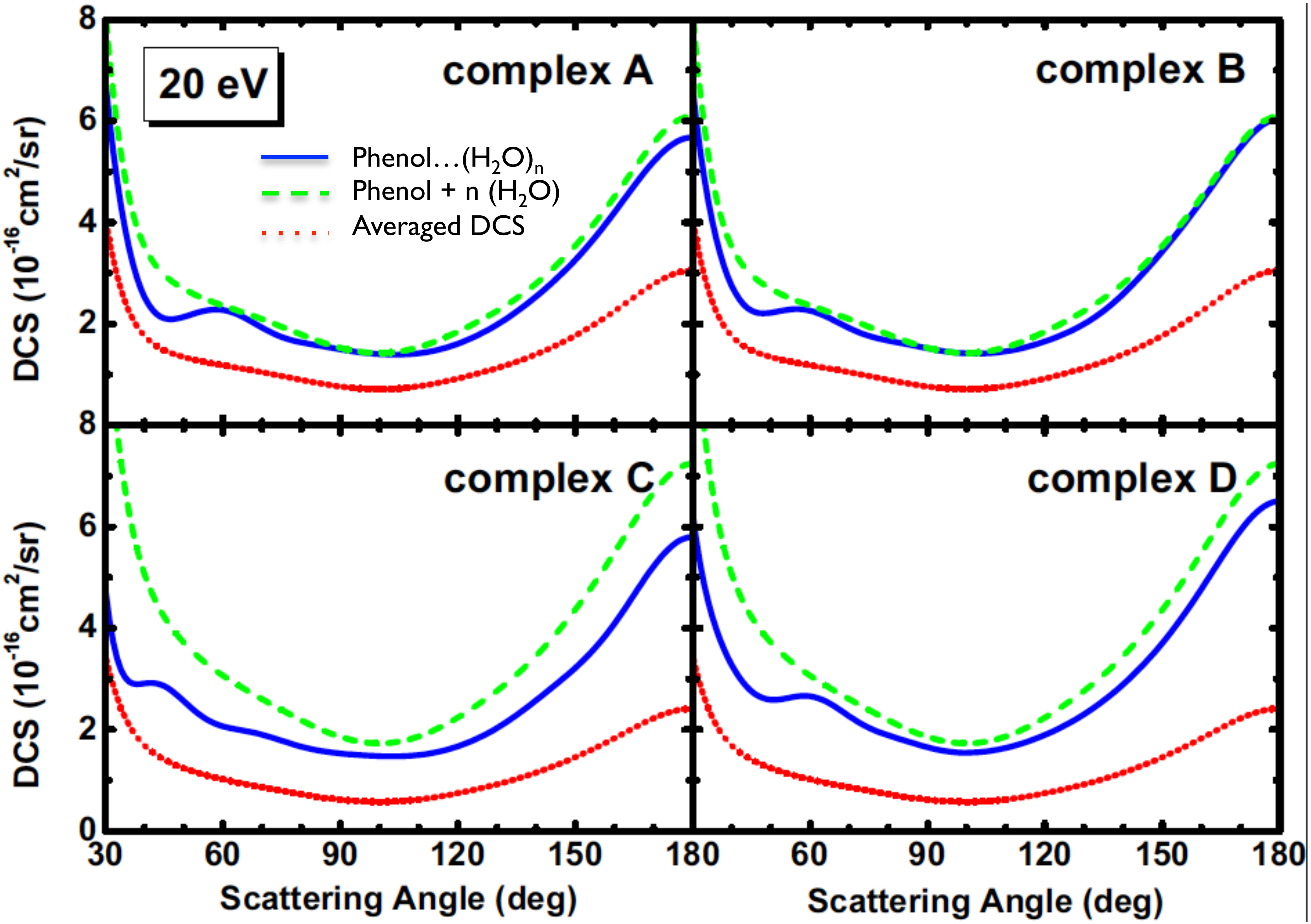
MAPLima

Electron Collisions with Phenol...$(H_2O)_n$: search for microsolvation signatures in the DCS



Electron Collisions with Phenol...$(H_2O)_n$: search for microsolvation signatures in the DCS



ELECTRONIC EXCITATION

Theoretical co-authors

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Márcio H. F. Bettega

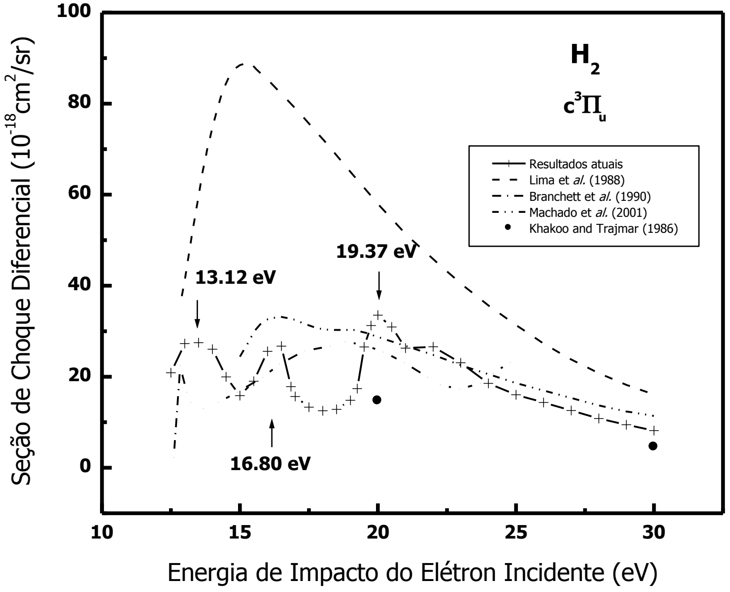
Márcio T. do N. Varella

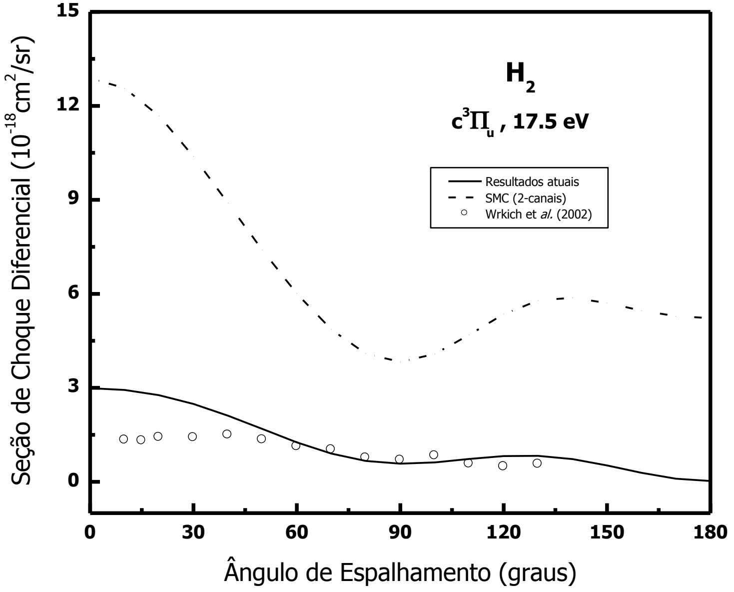
Universidade Federal do ABC

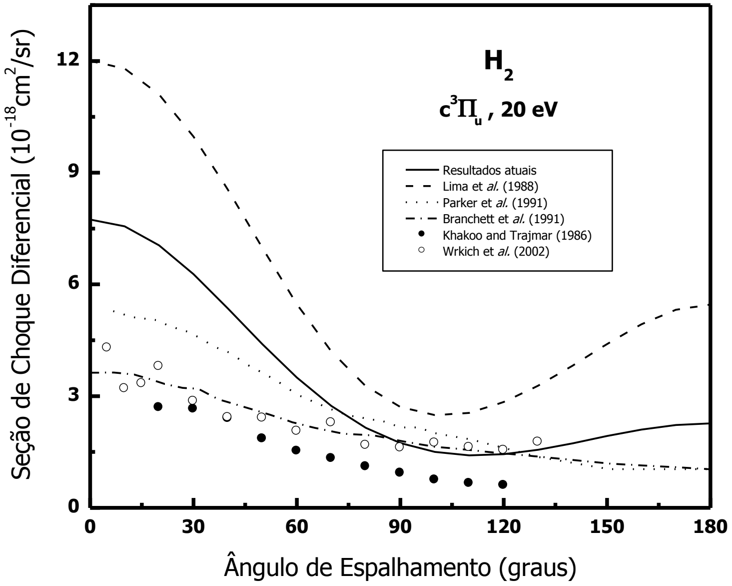
Romarly F. da Costa (coordinator)

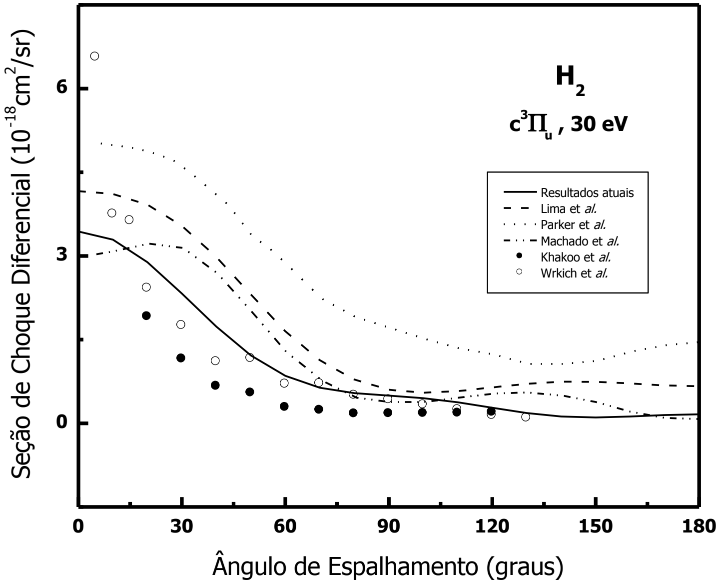
Electronic excitation of H_2 by electron impact

R. F. da Costa, F. J. da Paixão and M.A. P. Lima,
J. Phys. B **38**, 4363 (2005)



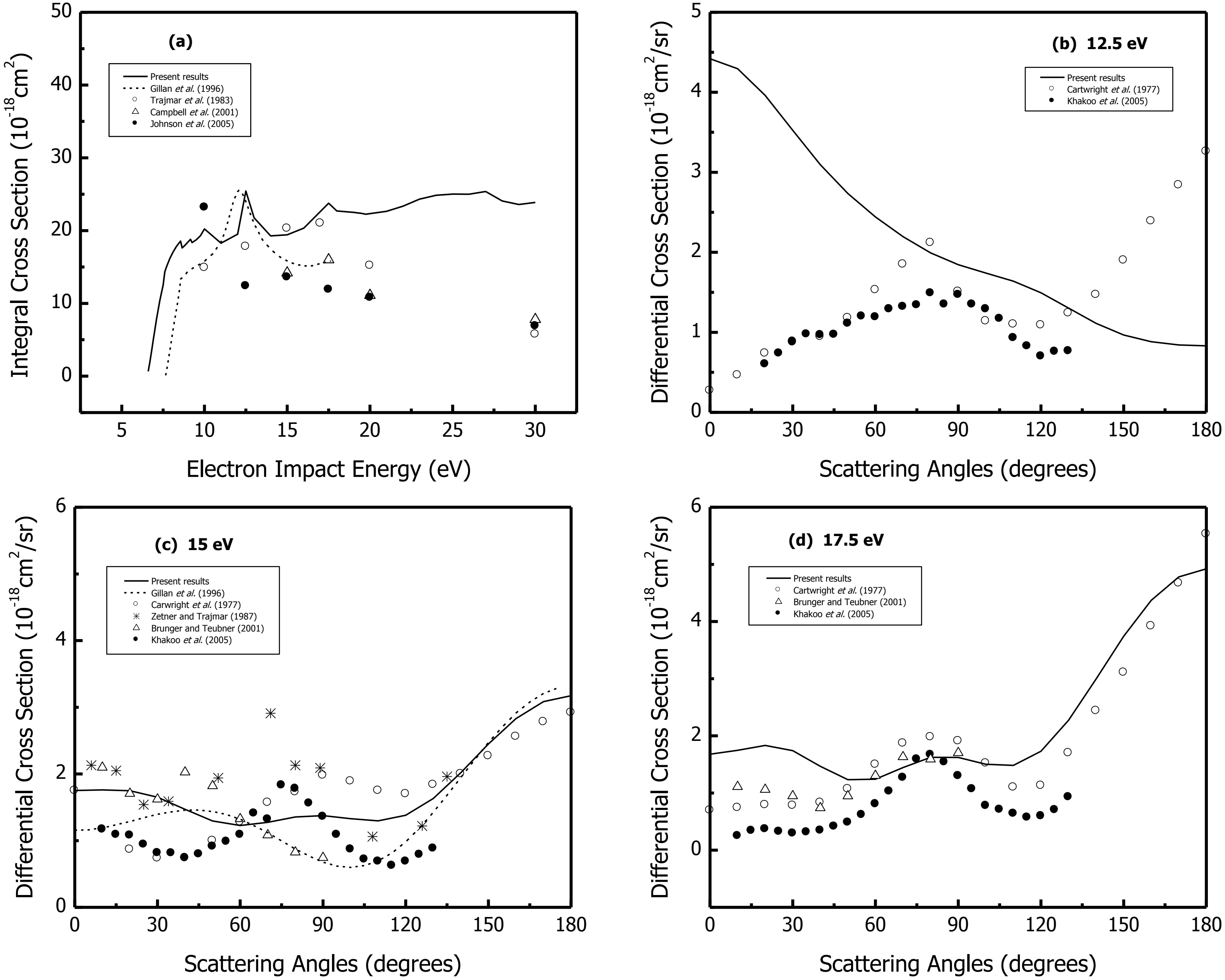






Electronic transition X $^1\Sigma_g \rightarrow$ A $^3\Sigma_u^+$ of N_2 by electron impact

R.F. da Costa and M.A. P. Lima,
Phys. Rev.A **75**, 022705 (2007)



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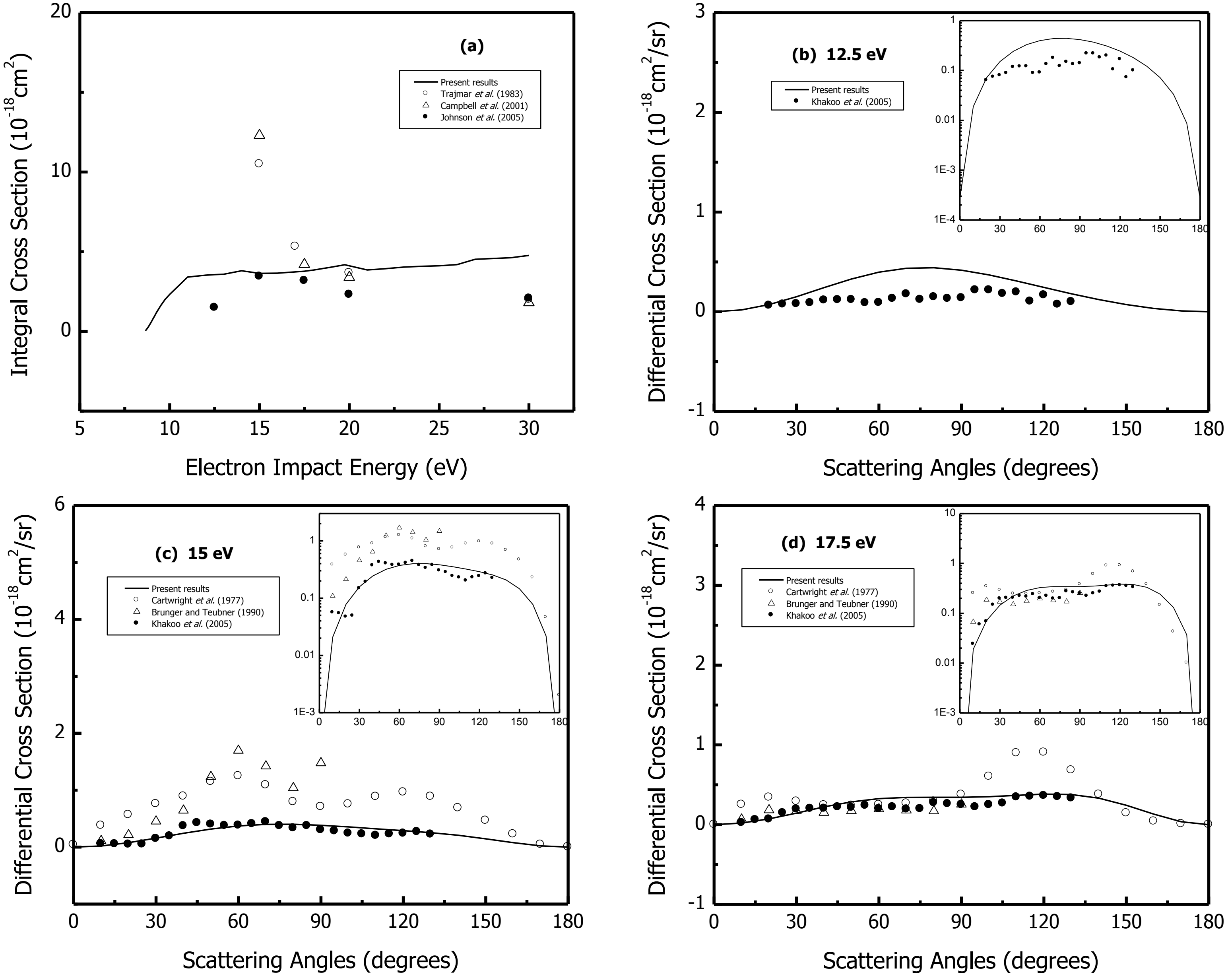
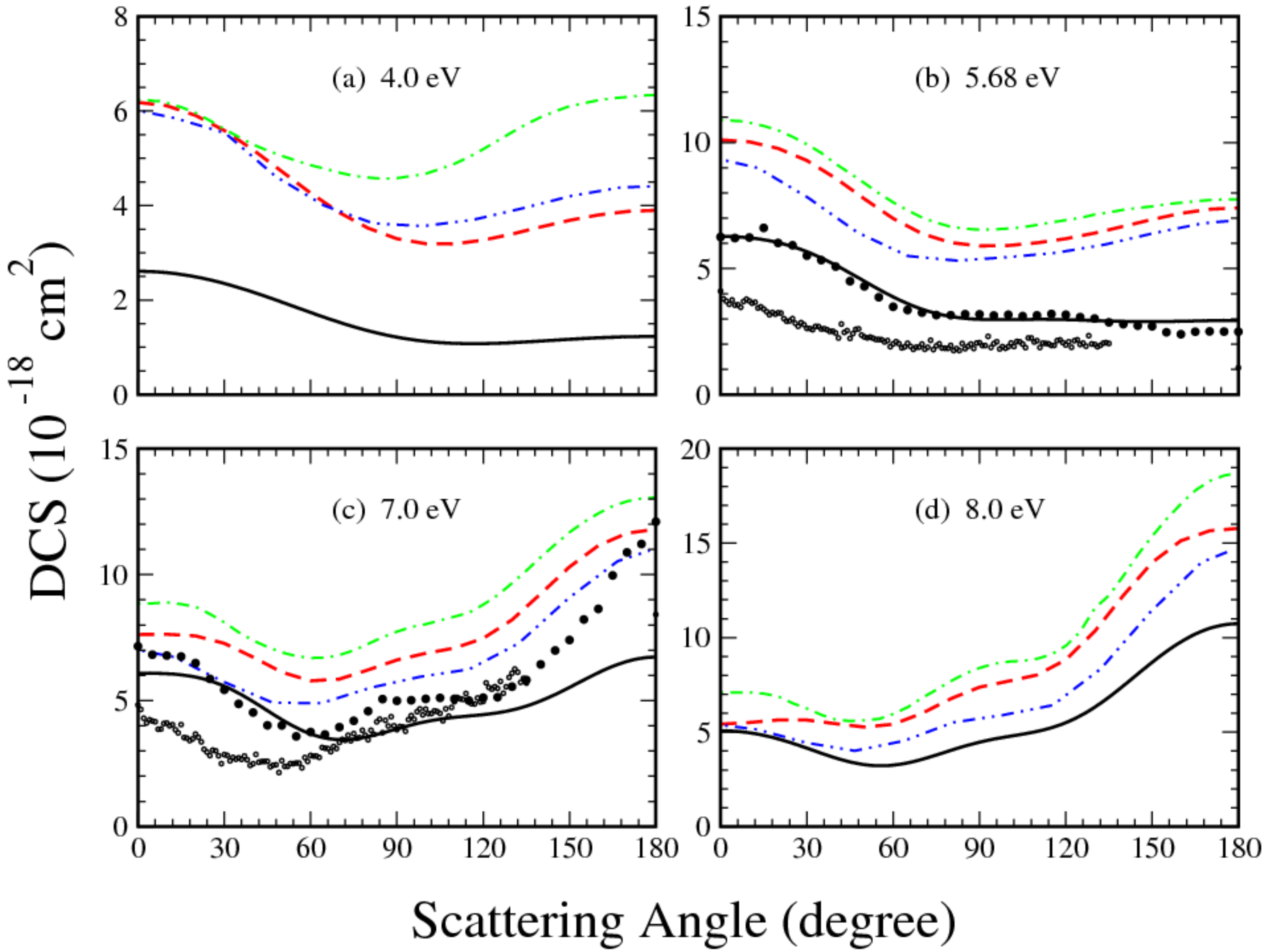
Electronic transition X $^{1}\Sigma_g \rightarrow$ a' $^{1}\Sigma_u^-$ of N_2 by electron impact

R.F. da Costa and M.A. P. Lima,
Phys. Rev.A **75**, 022705 (2007)



Electronic excitation of ã $^3B_{1u}$ state of C_2H_4 by electron impact

R. F. da Costa, M. H. F. Bettega, and M. A. P. Lima, *Phys. Rev. A* **77**, 042723 (2008).



Color lines are Close-coupling Calculations and bullets are M. Allan´s data

R. F. da Costa, et al. *Phys. Rev. A* **85**, 062706 (2012).

Electron scattering by Furan: the lowest triplet state

ELECTRONIC EXCITATION OF GAS-PHASE FURAN . . . PHYSICAL REVIEW A **85**, 062706 (2012)

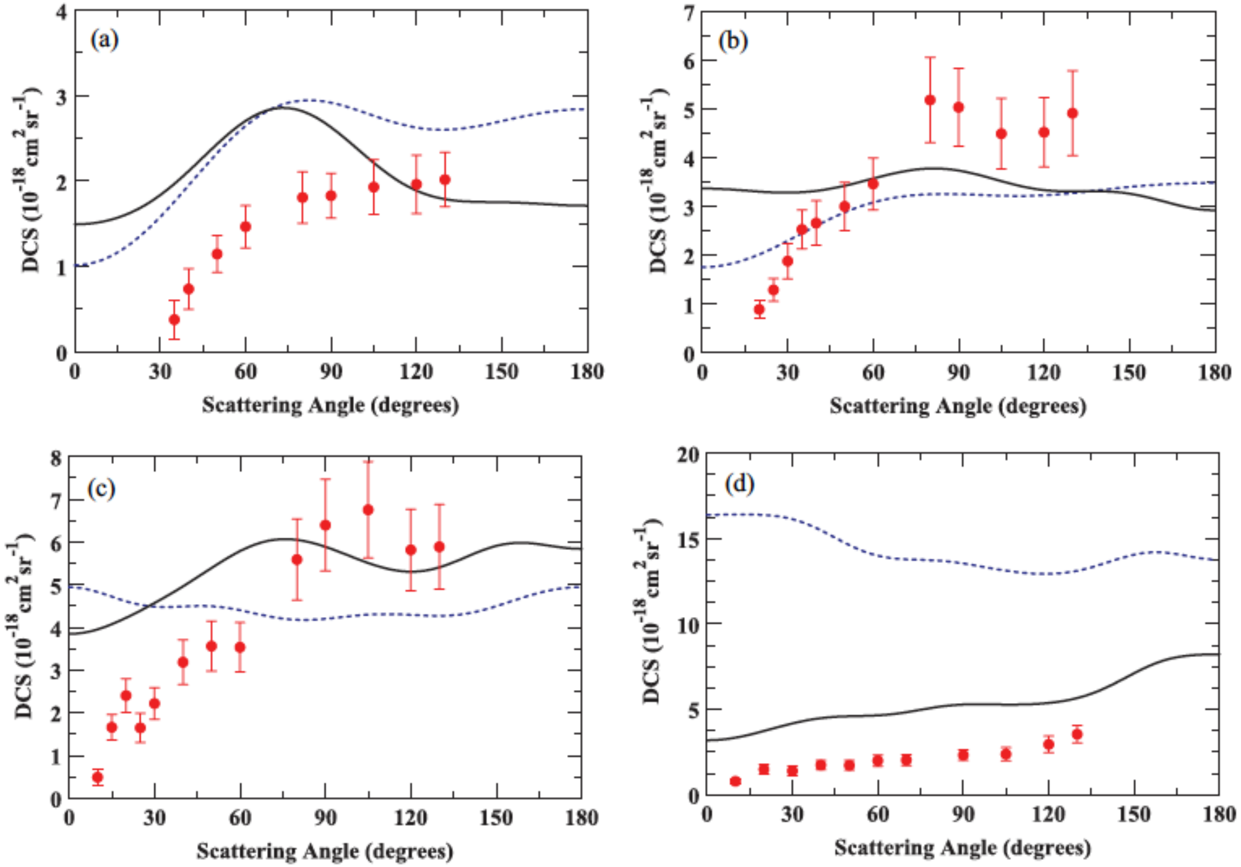


FIG. 6. (Color online) Differential cross section for the electronic excitation from ground state to the $^3B_2$ state of furan by electron impact at an energy of (a) 5 eV, (b) 6 eV, (c) 7.5 eV, and (d) 10 eV. The present experimental data (solid circles) are shown, as well as the present theoretical results from model 1 (black solid curve) and model 2 (blue dashed curve).

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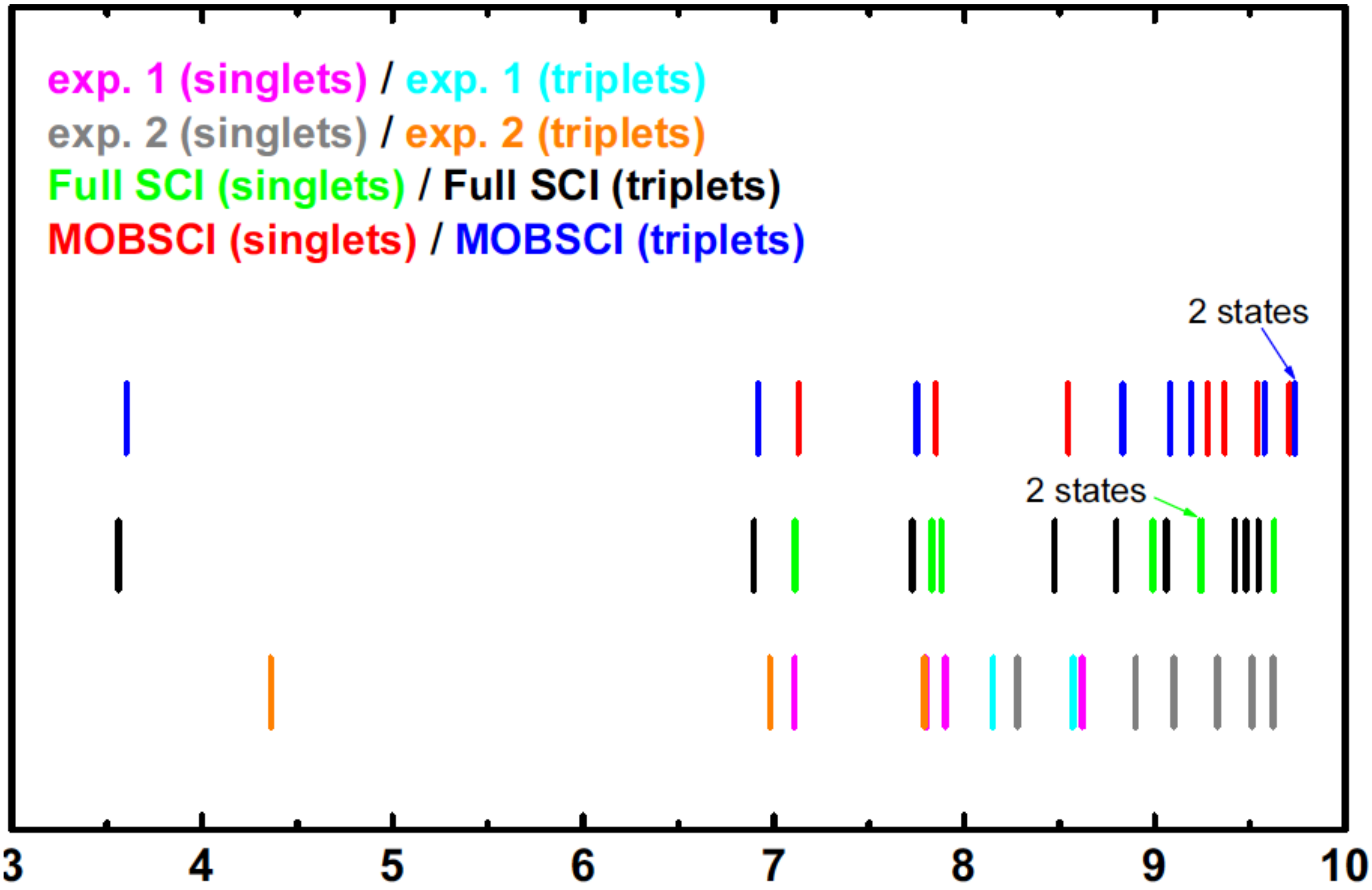
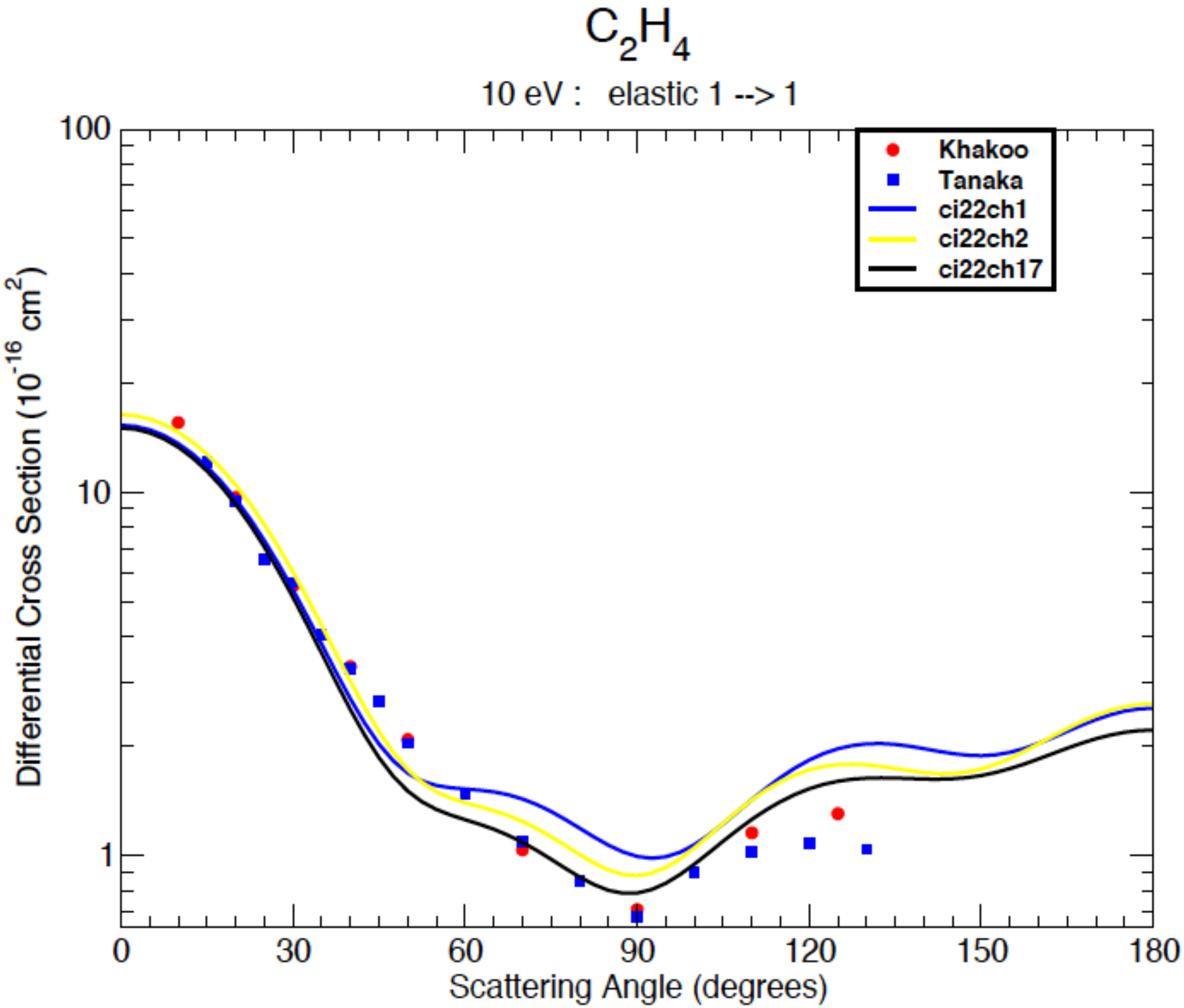
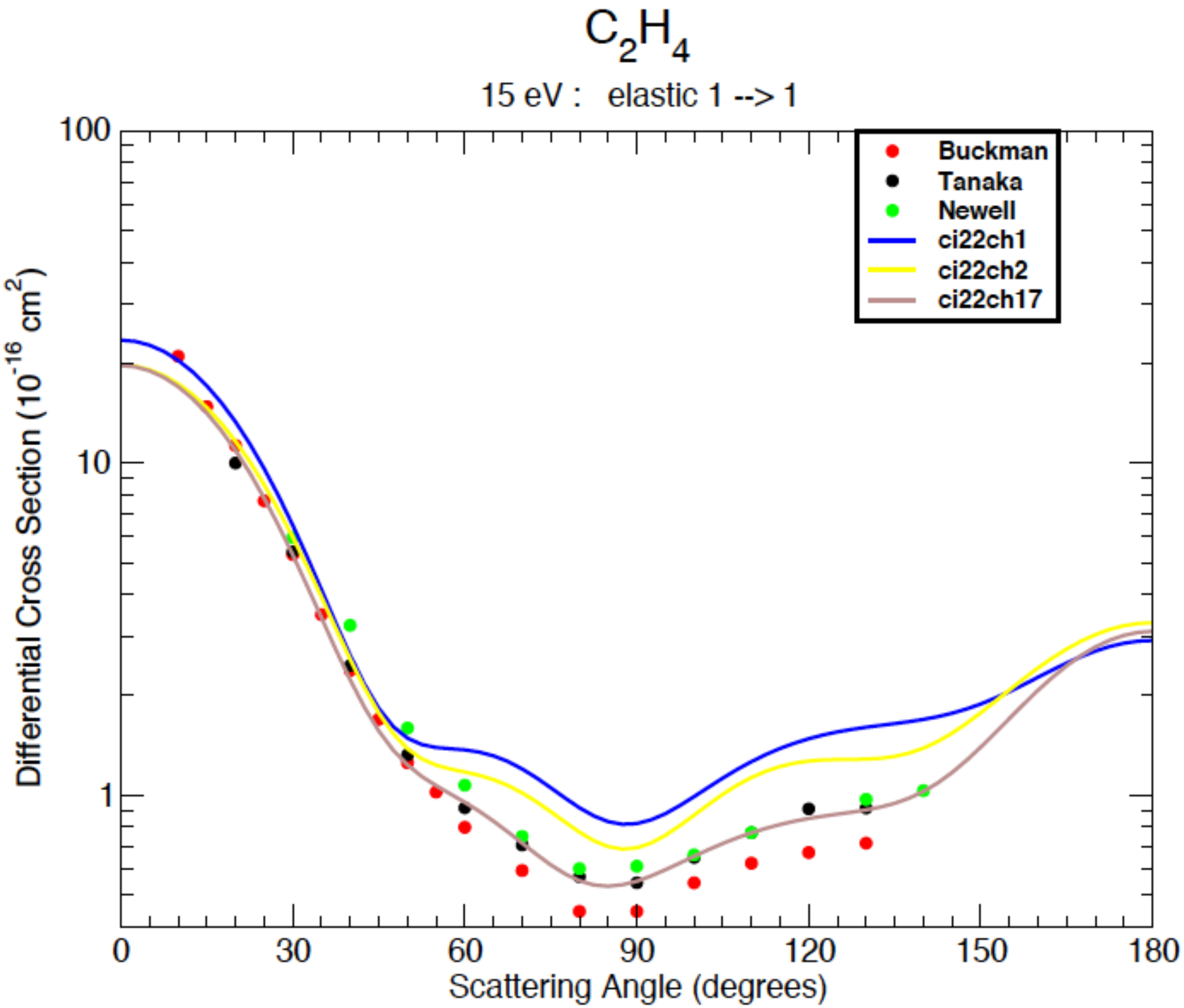
Multichannel effects on the e^--C_2H_4 scattering



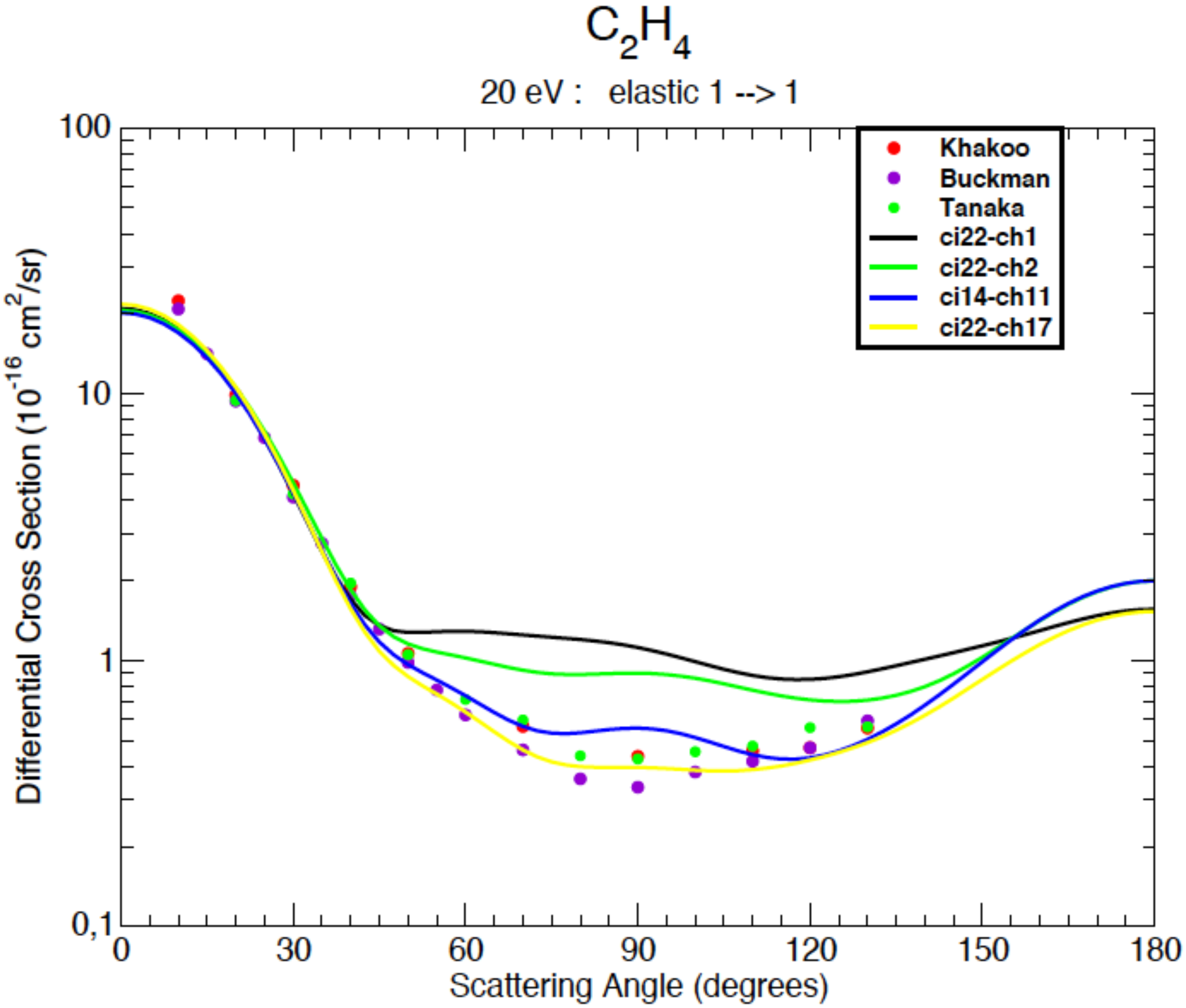
Multichannel effects on the elastic process of e$^-$-C_2H_4 scattering



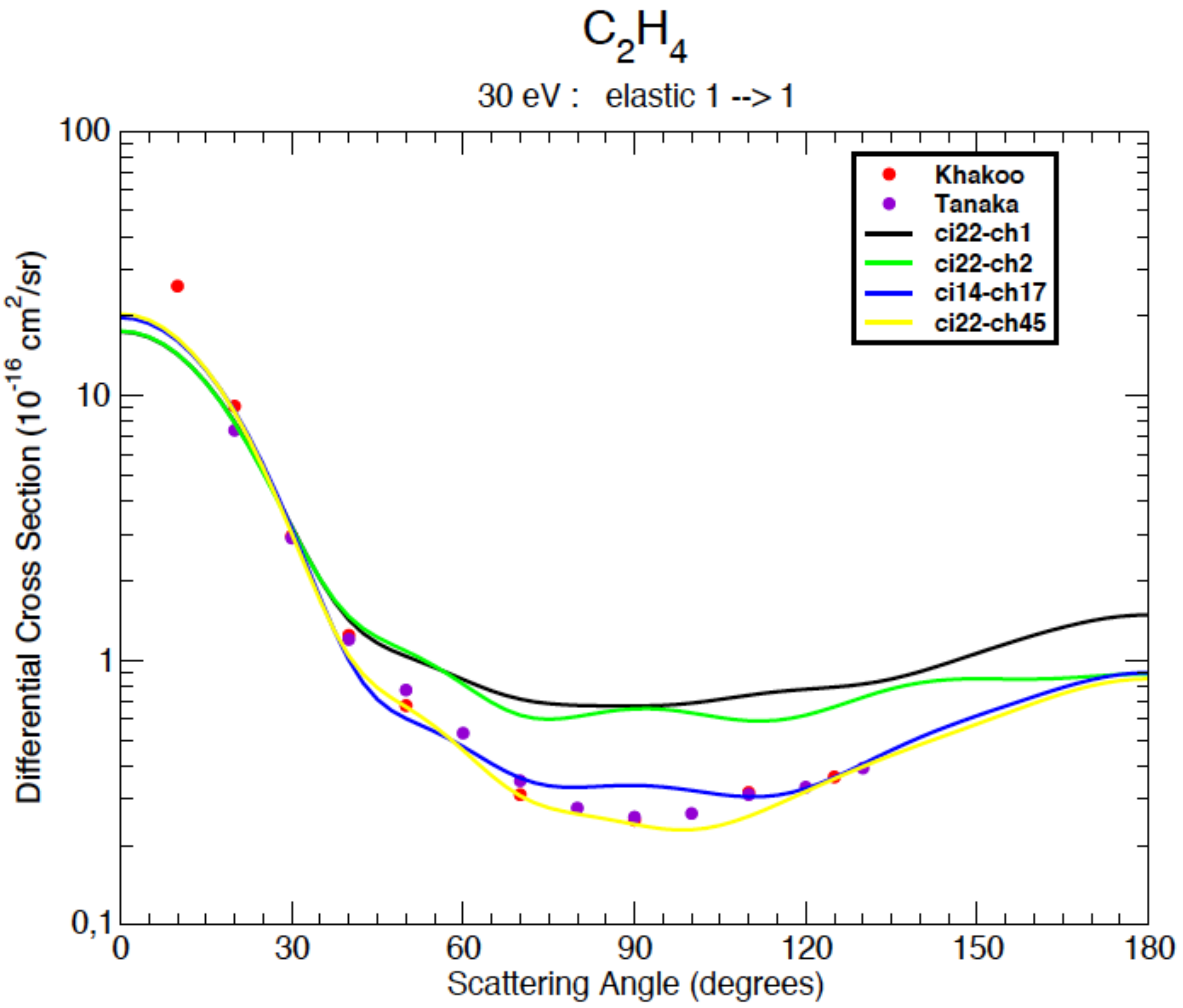
Multichannel effects on the elastic process of e$^-$-C_2H_4 scattering



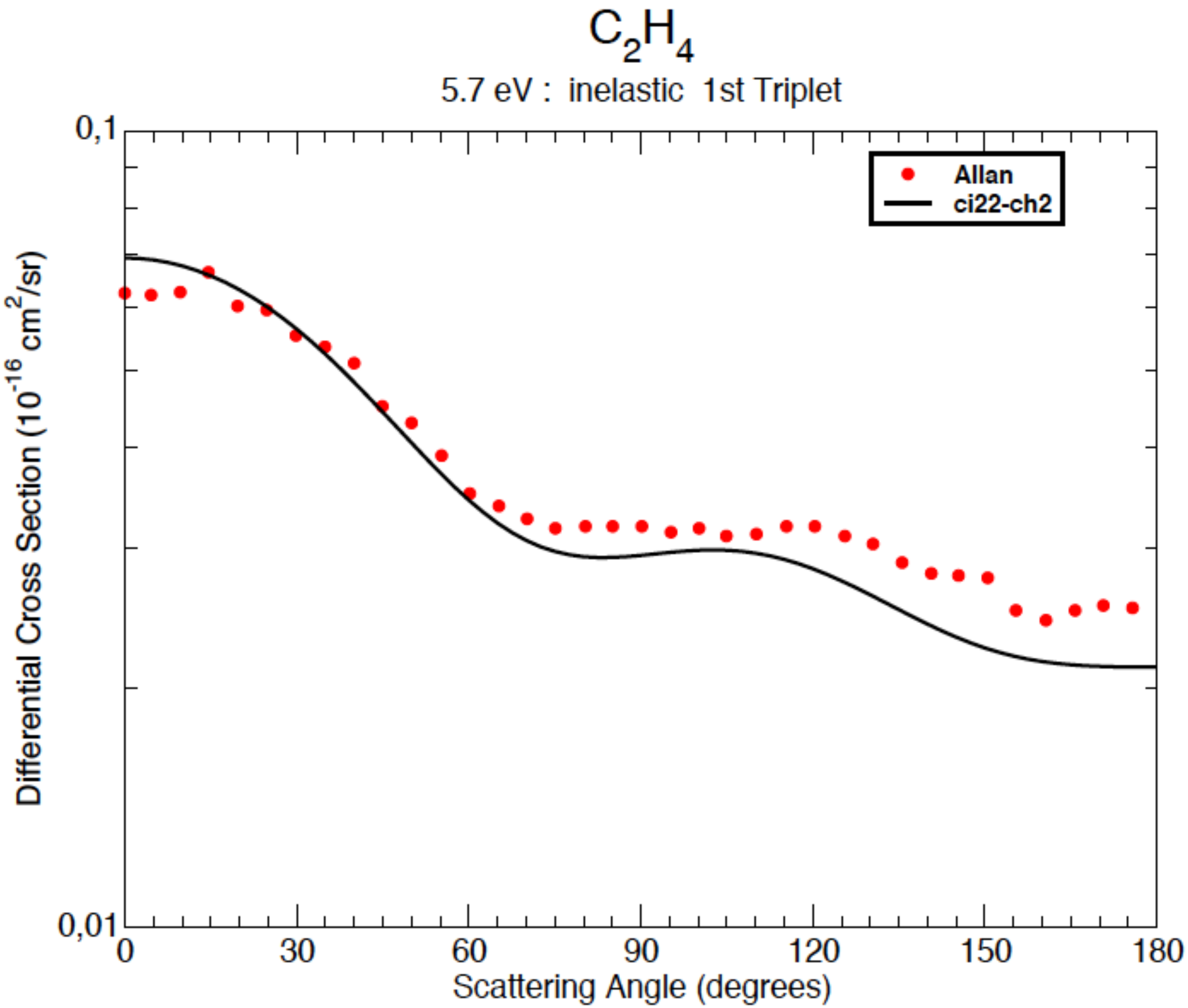
Multichannel effects on the elastic process of e^{-}-C_2H_4 scattering



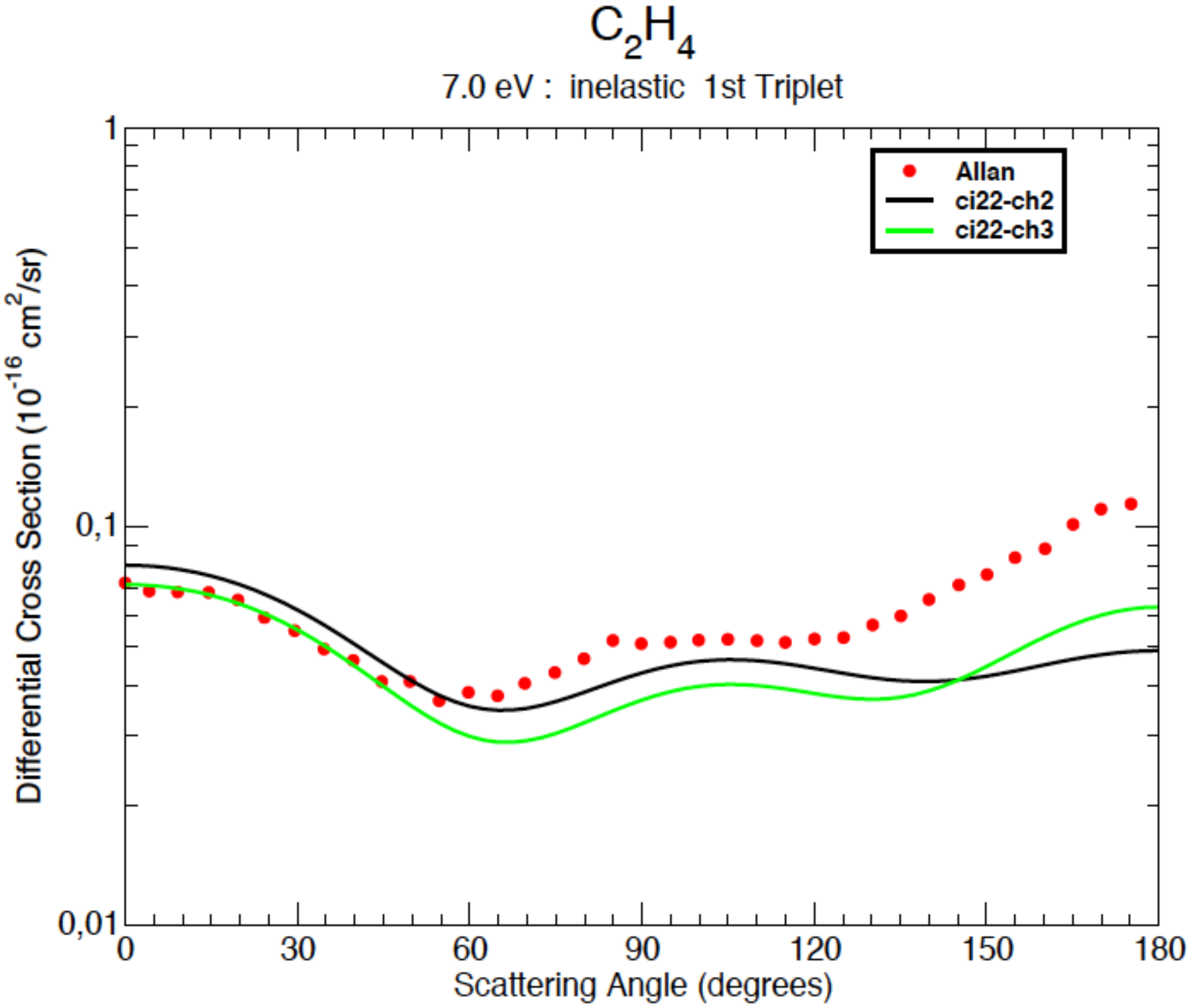
Multichannel effects on the elastic process of e^--C_2H_4 scattering



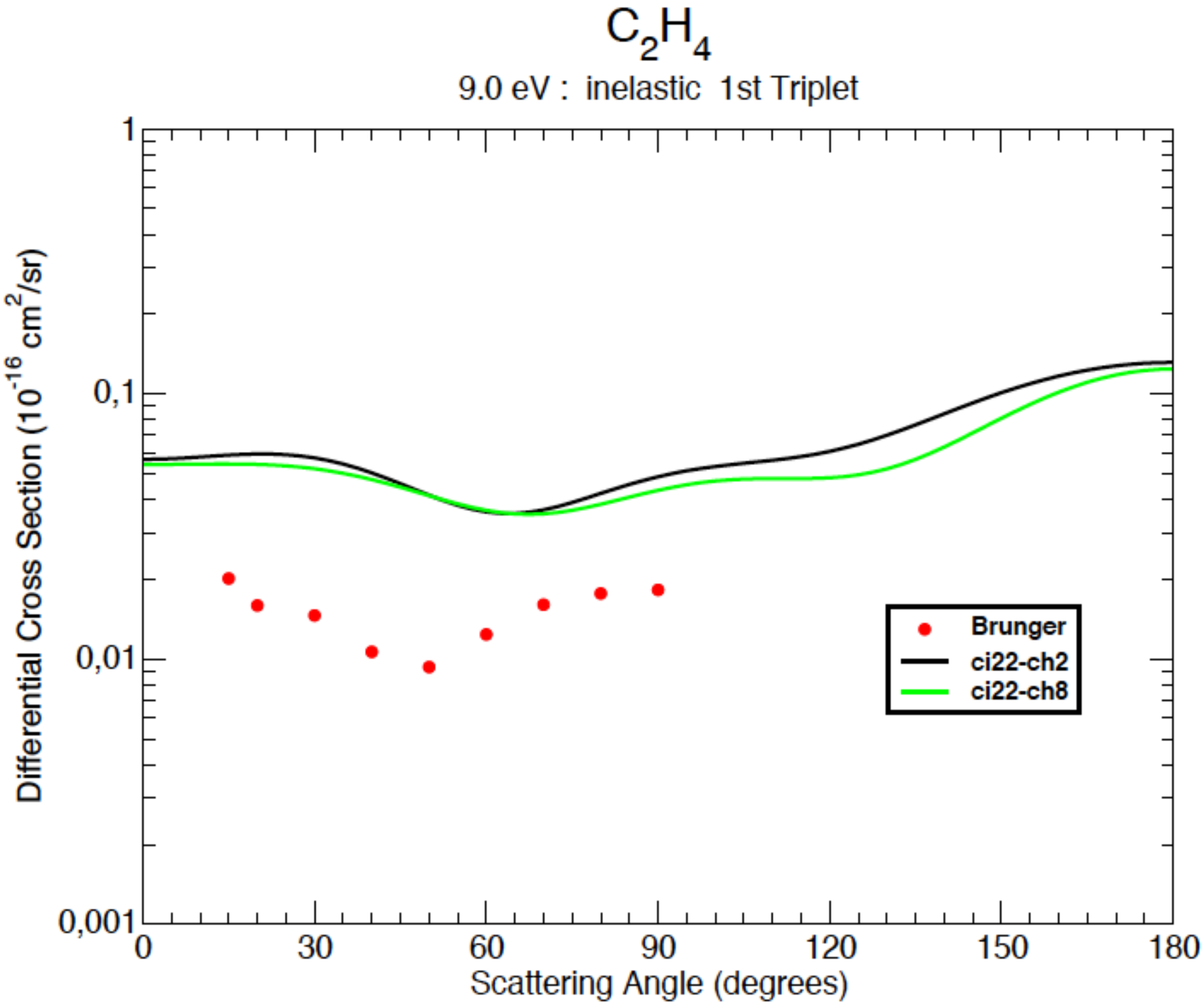
Multichannel effects on the Electronic excitation of ã $^3B_{1u}$ state of C_2H_4 by electron impact



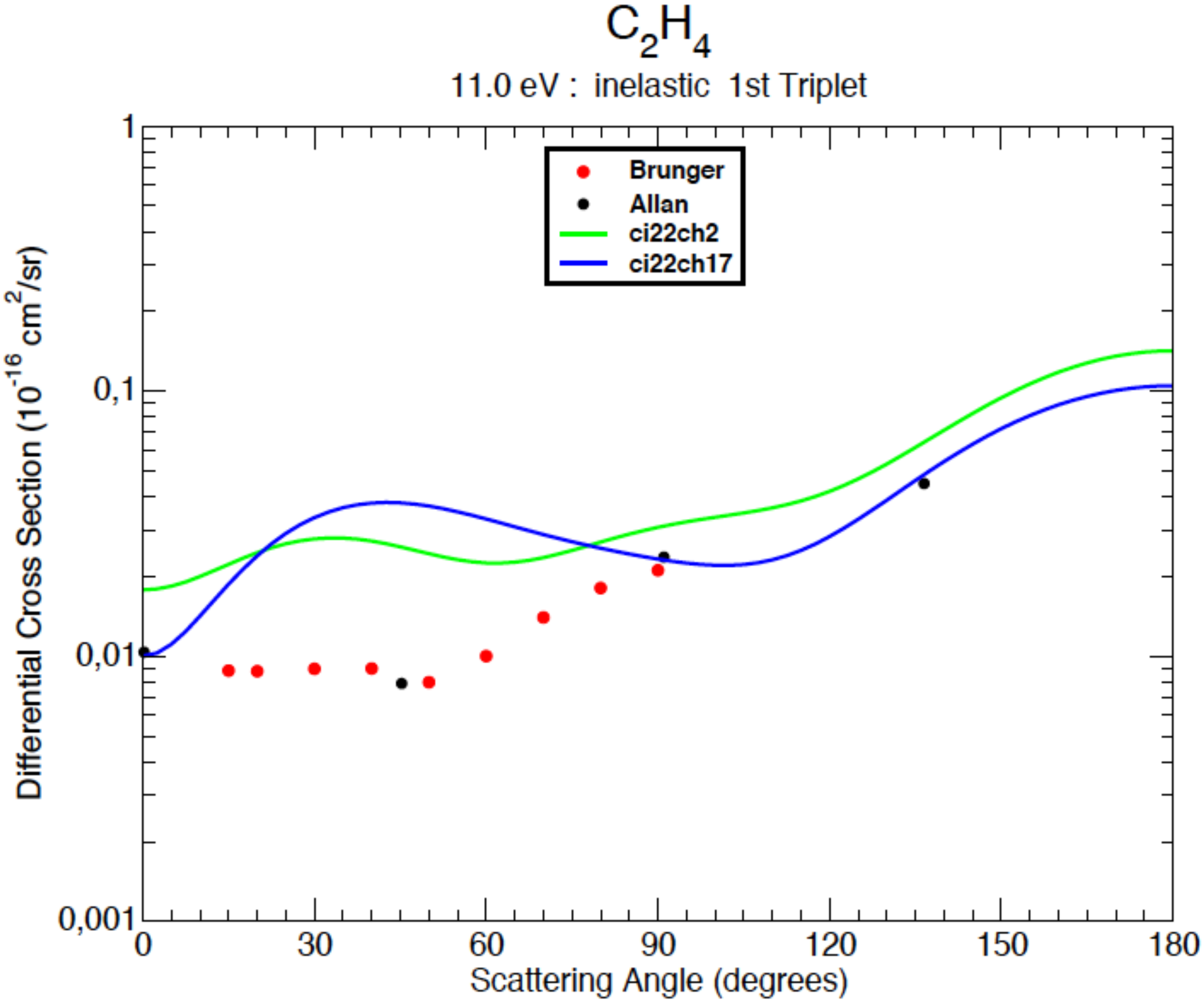
Multichannel effects on the Electronic excitation of ã $^3B_{1u}$ state of C_2H_4 by electron impact



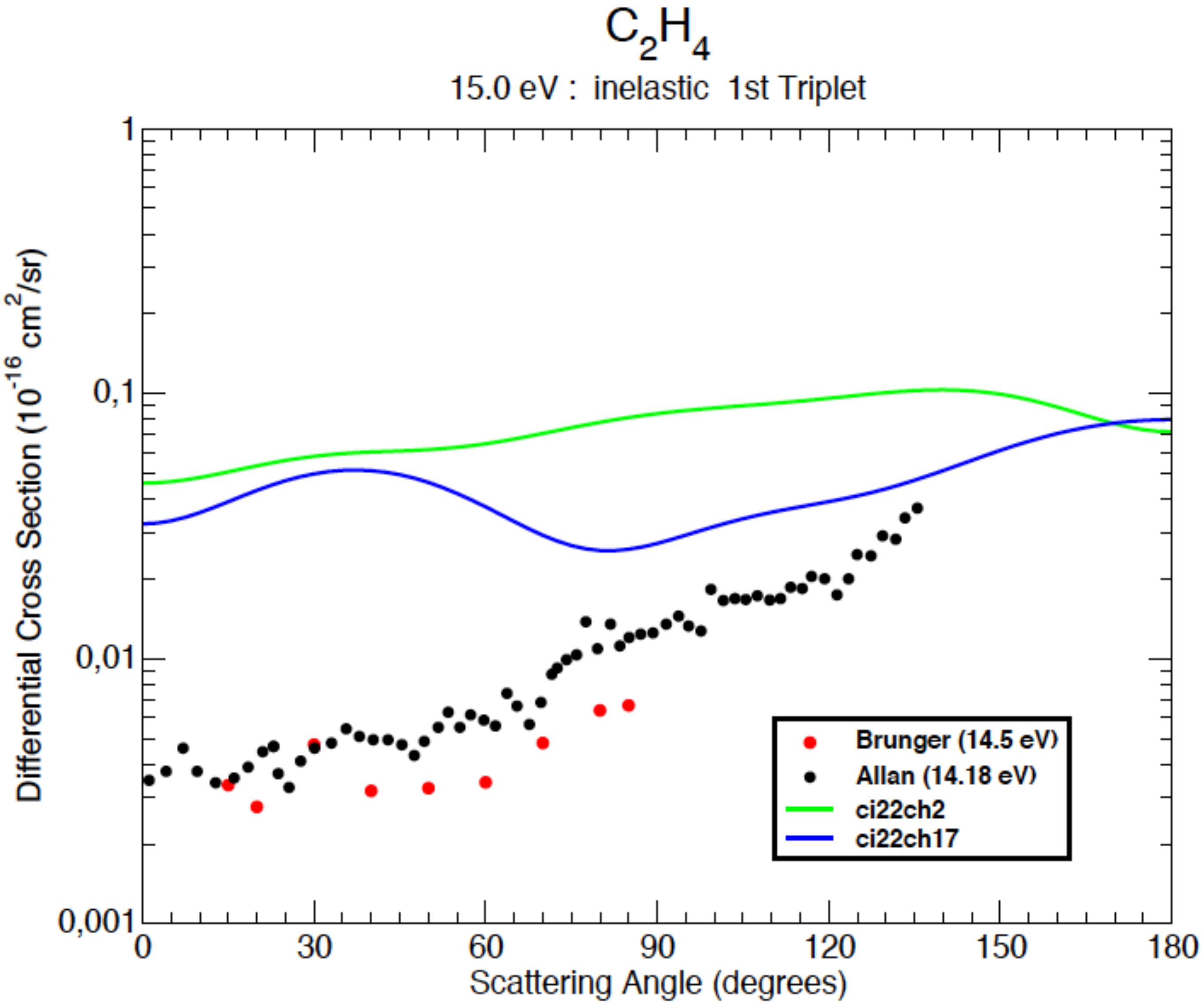
Multichannel effects on the Electronic excitation of ã $^3B_{1u}$ state of C_2H_4 by electron impact



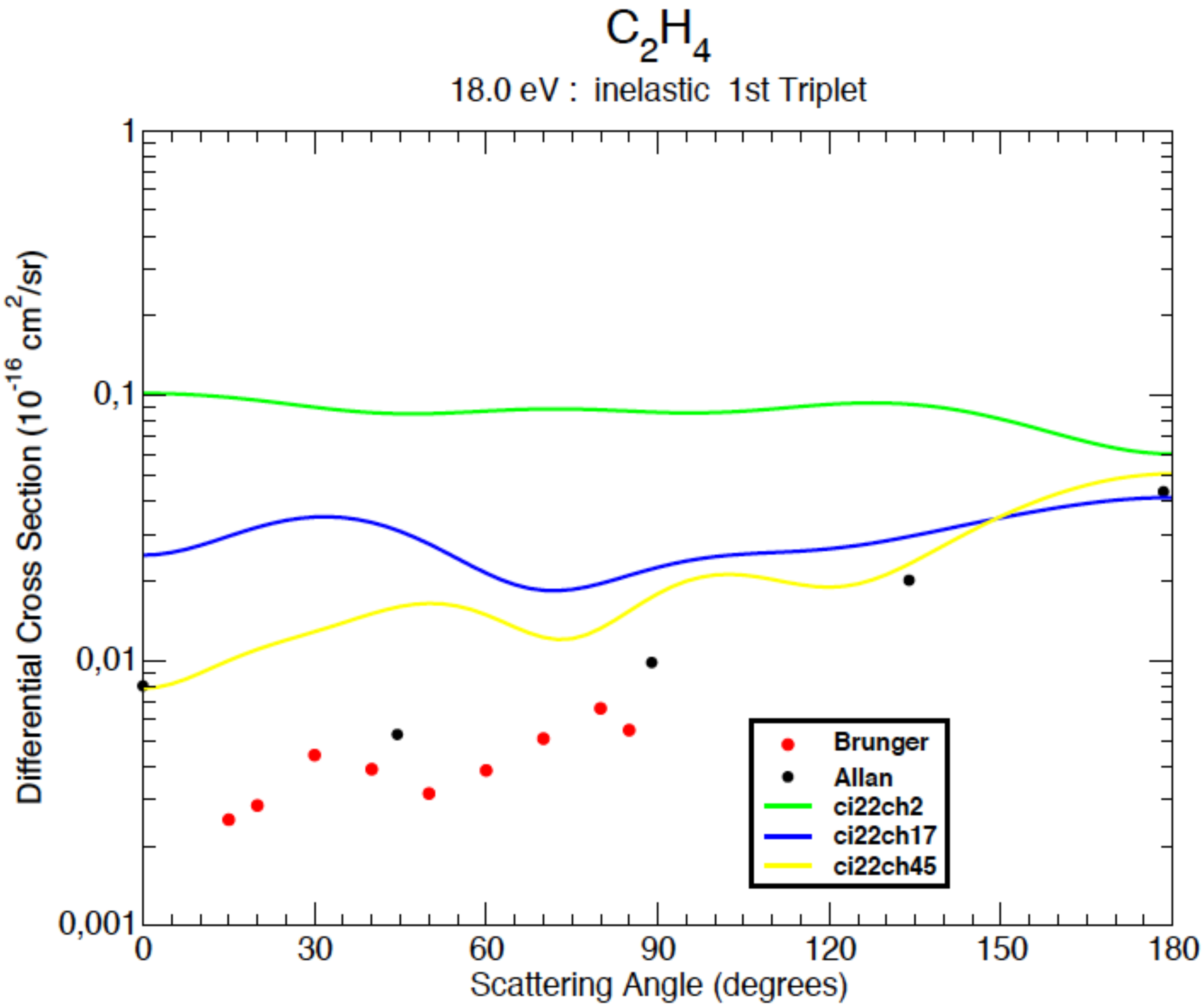
Multichannel effects on the Electronic excitation of ã $^3B_{1u}$ state of C_2H_4 by electron impact



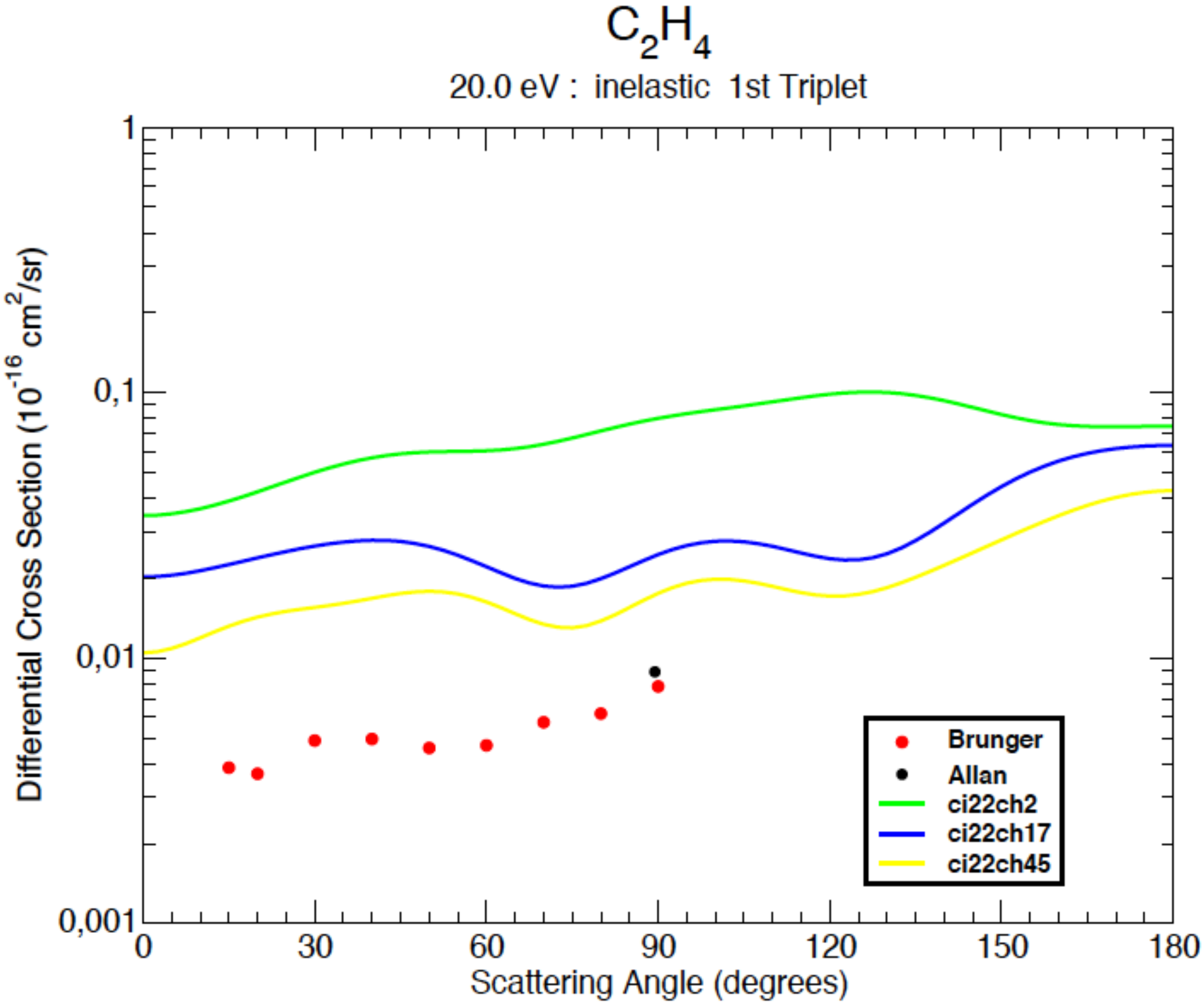
Multichannel effects on the Electronic excitation of ã $^3B_{1u}$ state of C_2H_4 by electron impact



Multichannel effects on the Electronic excitation of ã $^3B_{1u}$ state of C_2H_4 by electron impact



Multichannel effects on the Electronic excitation of ã $^3B_{1u}$ state of C_2H_4 by electron impact



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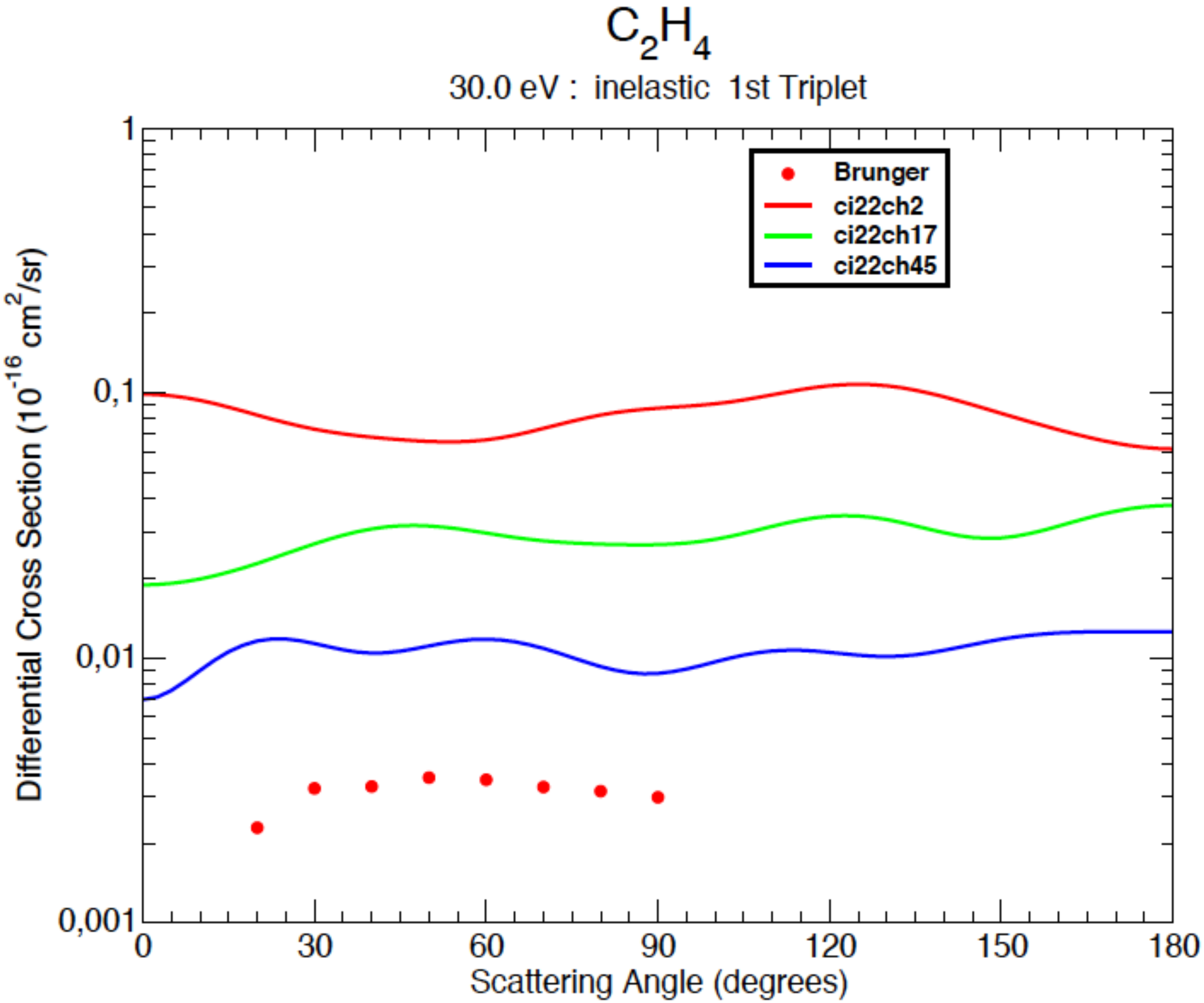
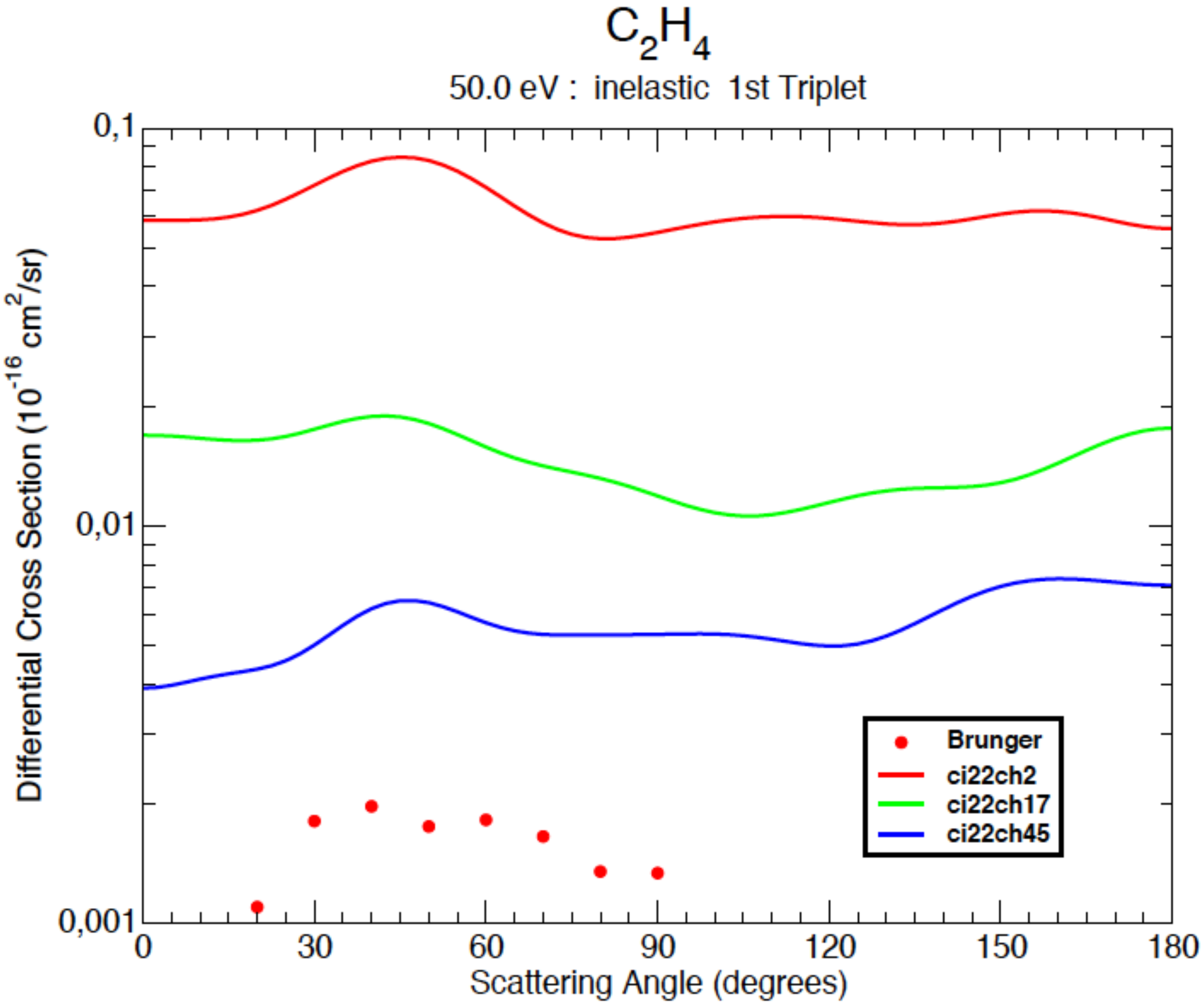


Multichannel effects on the Electronic excitation of ã $^3B_{1u}$ state of C_2H_4 by electron impact



Thank you very much for your attention

A copy of this presentation is at
http://www.ifi.unicamp.br/~maplima/maplima-IFT2014.pdf