Low energy electron scattering data for chemical plasma treatment of biomass

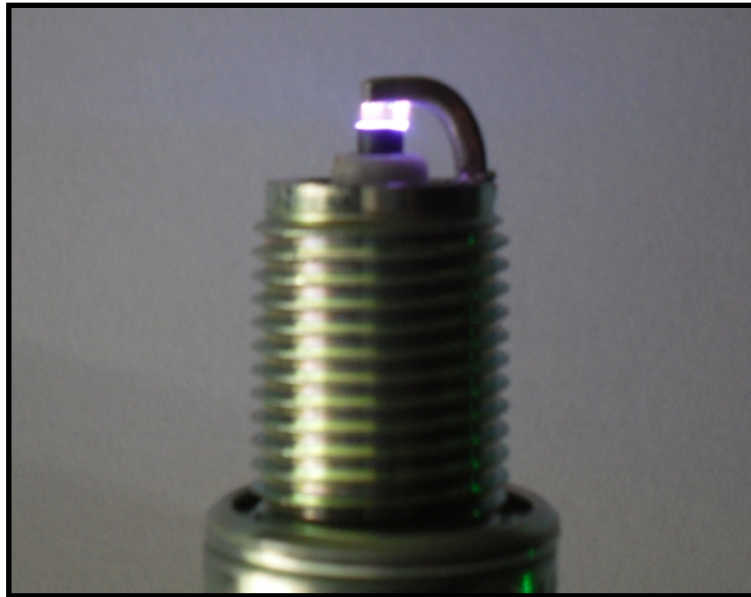by

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1

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Motivation I: large scale use of ethanol in engines
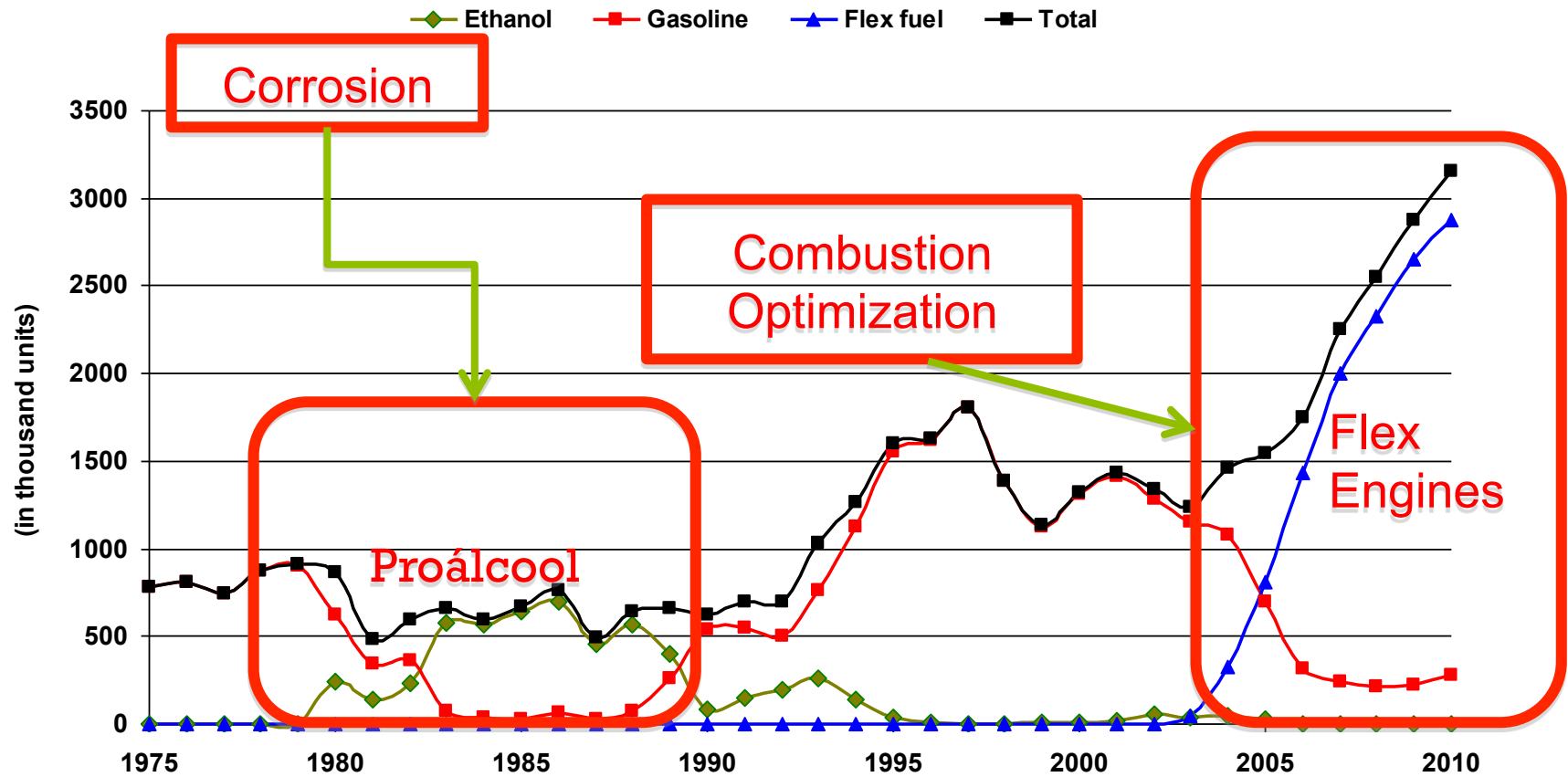
Brazilian Sales of light fleet Vehicles (1975-2010)

# 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)
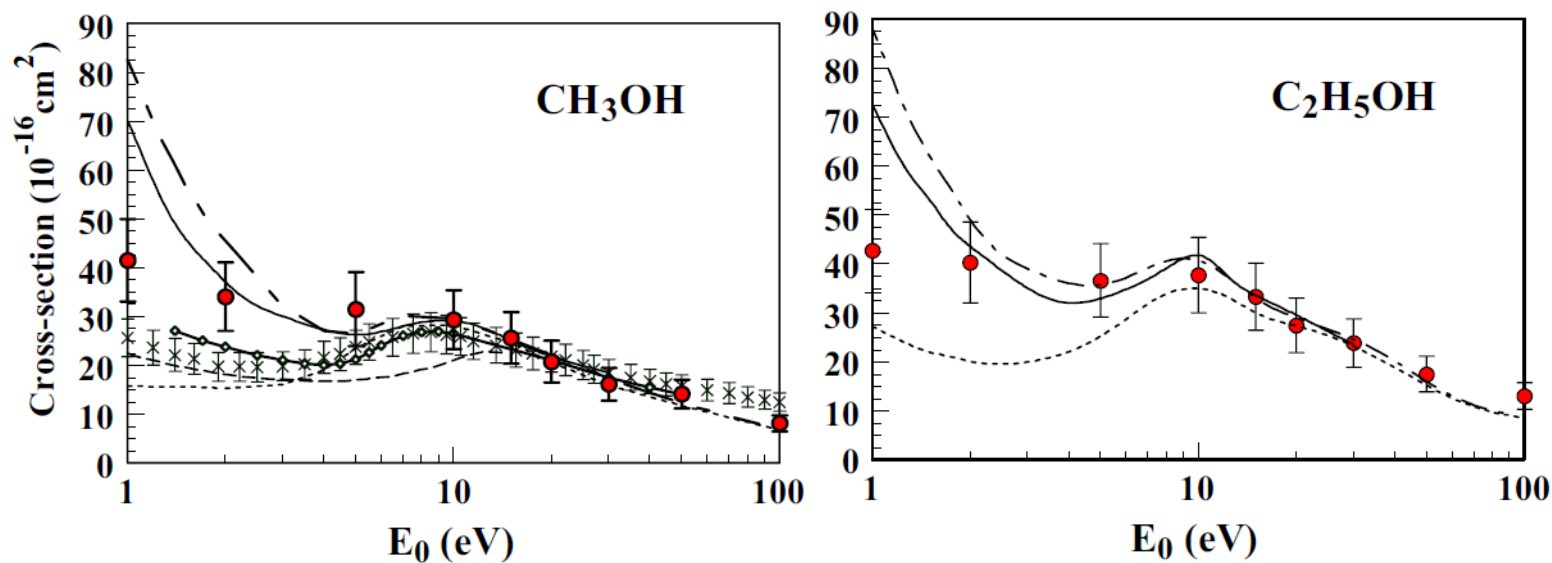
Integral elastic scattering cross sections for CH_3OH. Legend: ●: present experiment; ———: SMCPP SEP; —: SMC SEP; ---- (short dashes): SMC SE which is similar to SMCPP SE; and ---- (long dashes): R-matrix ICSs of Bouchiha et al. (without Born correction) [10]. × Total cross section measurements of Szmytkowski and Krzysztofowicz [24] and —◆— of Schmieder [22]. ----- (short dashes) are from the SMCPP SE which is similar to SMC SE.
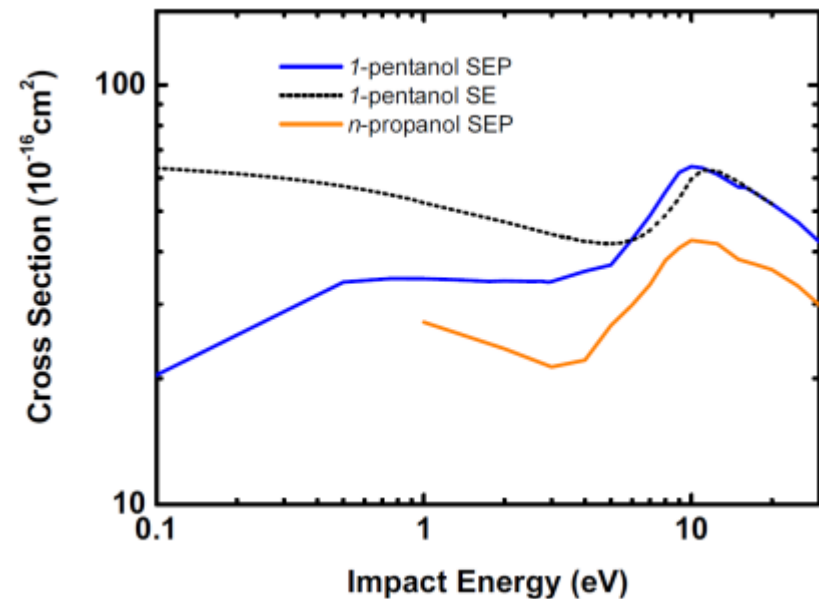
NSF/CNPq project (experiments from Morty Khakoo's group)

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

PHYSICAL REVIEW A **78**, 062714 (2008)
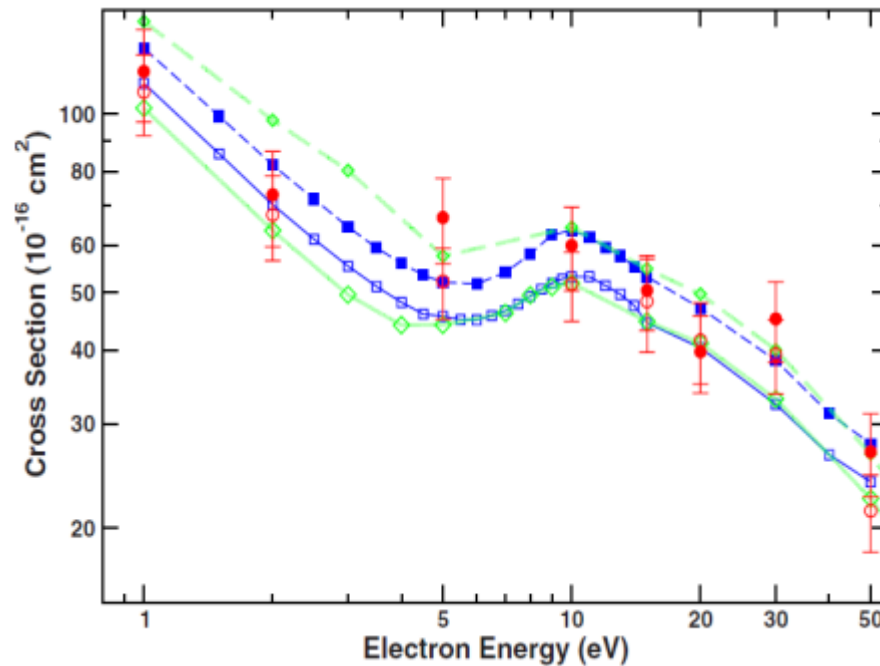
Electron scattering of slow electrons by *1*-pentanol (a drop in fuel)

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)

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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

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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

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Funding Motivation

- 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)

- 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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Theoretical co-authors

Eliane M. de Oliveira (posdoc)
Alexandra Natalense
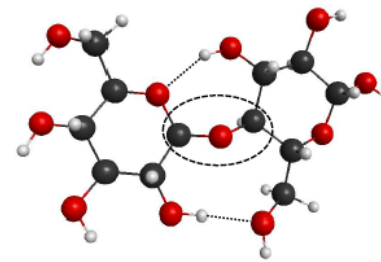Marco A. P. Lima

Sergio d'A. Sanchez
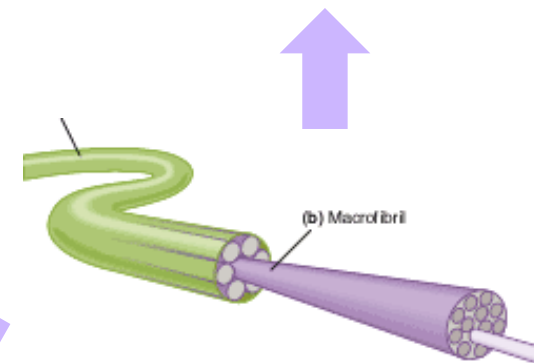Márcio H. F. Bettega

Romarly F. da Costa

Márcio T. do N. Varella (coordinator)

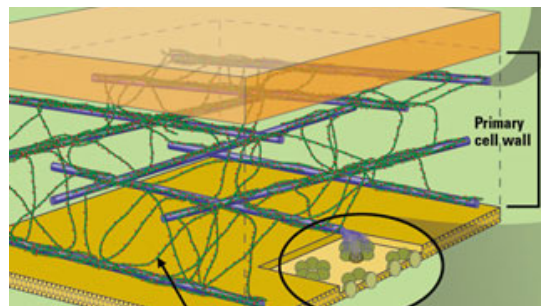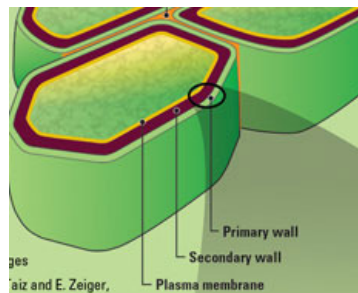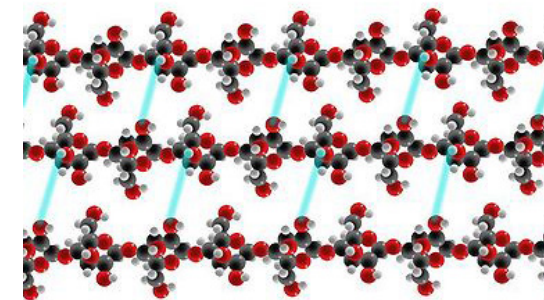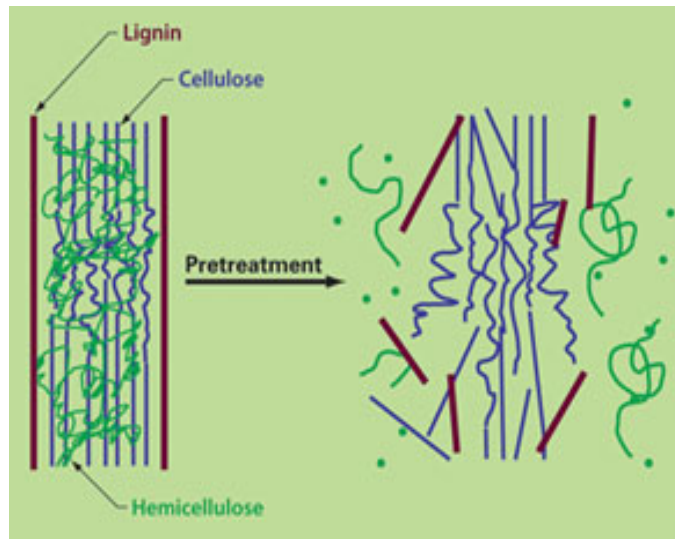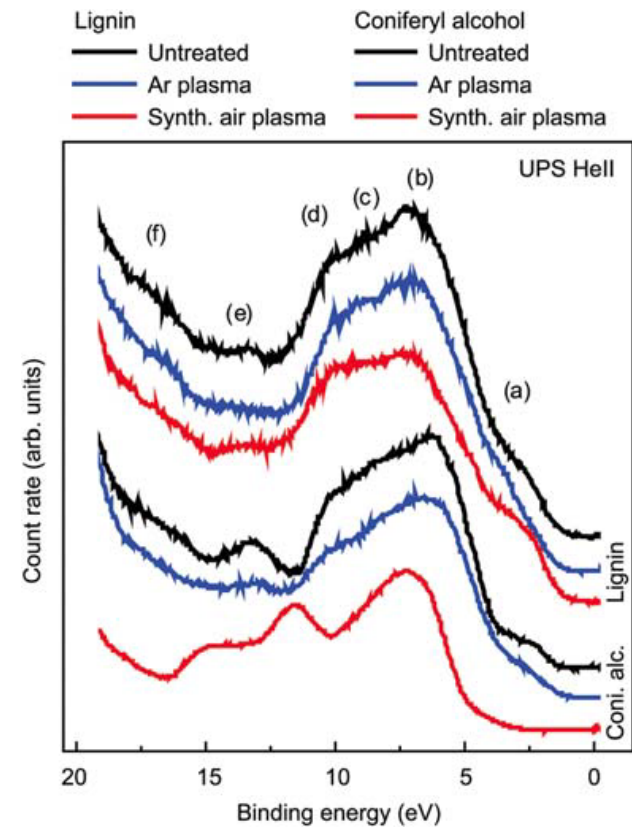# Biomass is Made Up with Fermentable Sugars
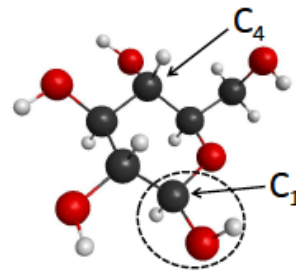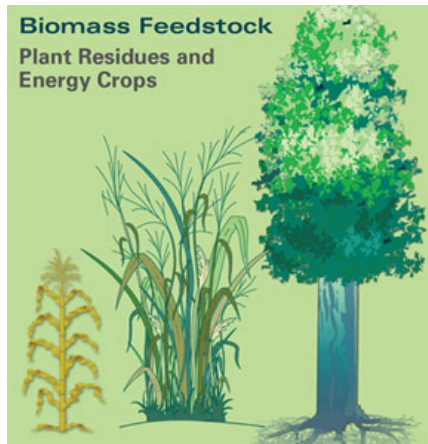
β-D-glucose

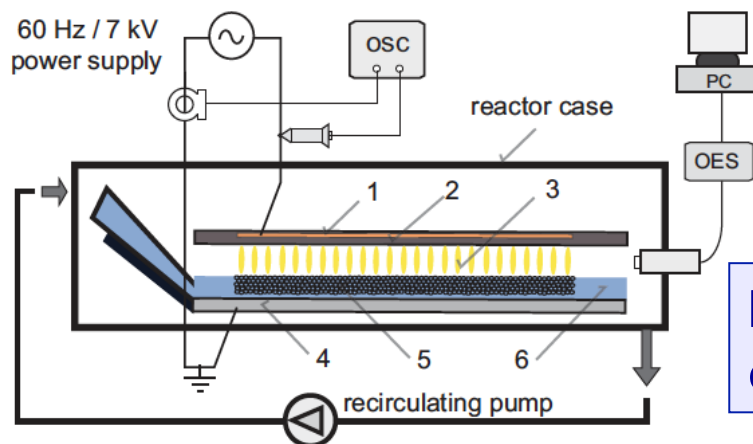cellobiose

Lignocellulose is Resistant to Hydrolysis

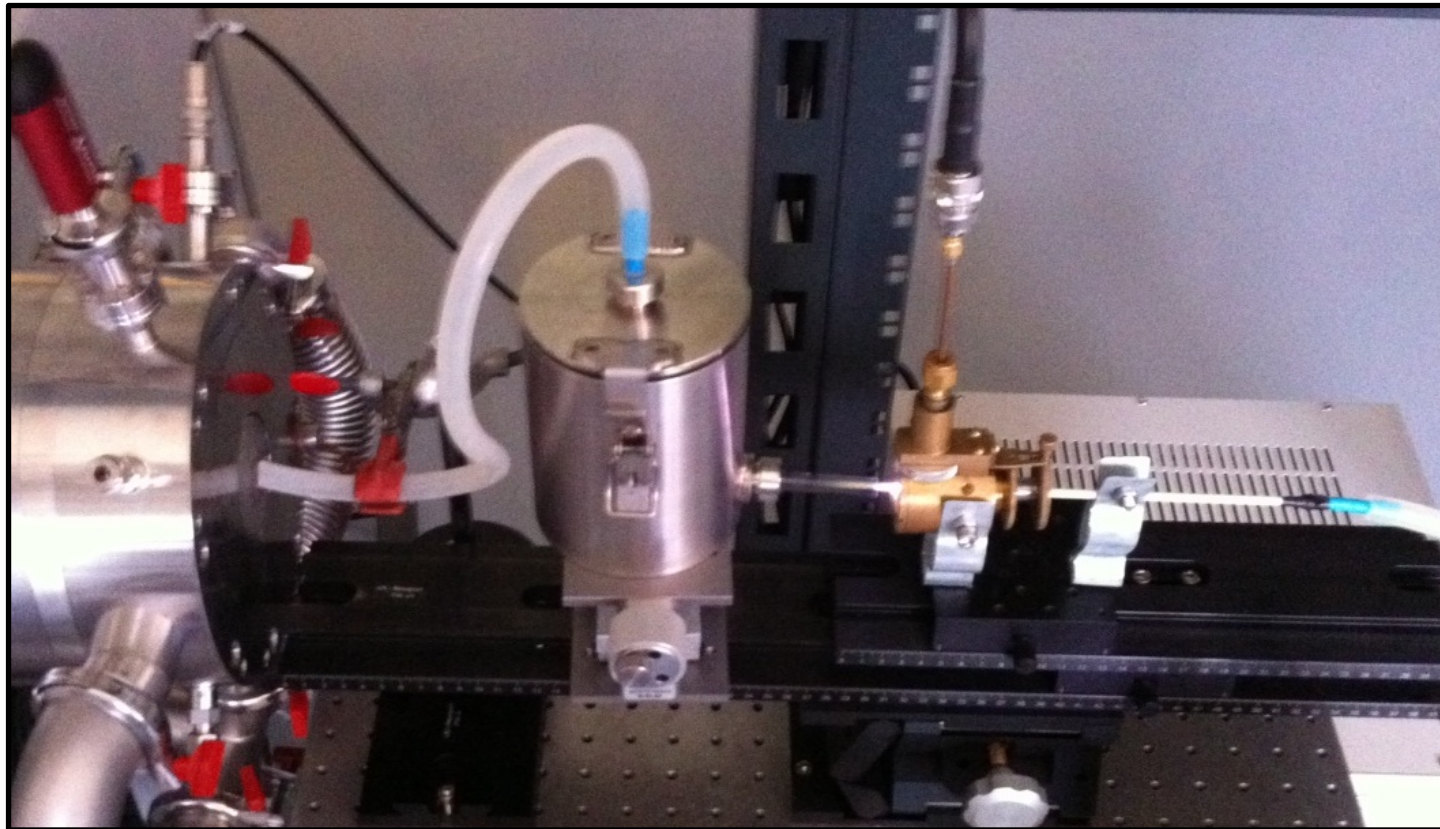**Pretreatment:** bio- and physical-chemical processes to expose the cellulose fibers

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

Dielectric Barrier Discharge (DBD): electron flux on substrate $\sim 10^8$ 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!!!

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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
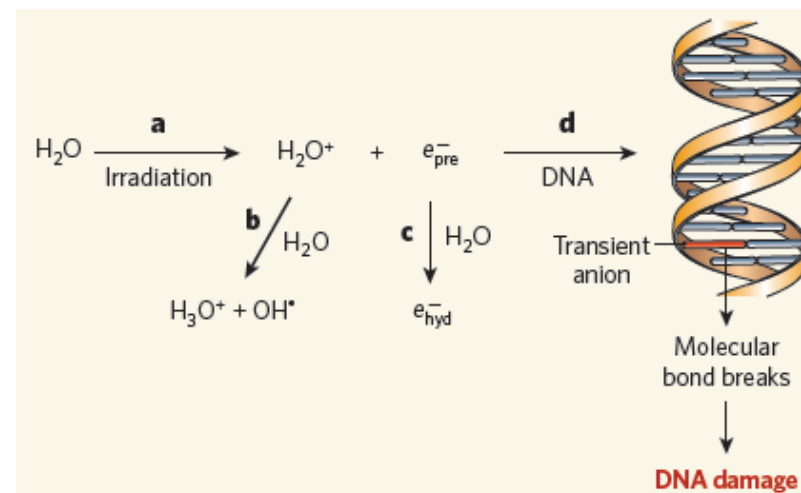
$$e^- + RH \rightarrow (RH)^{*-} \rightarrow R^\cdot + H^-$$
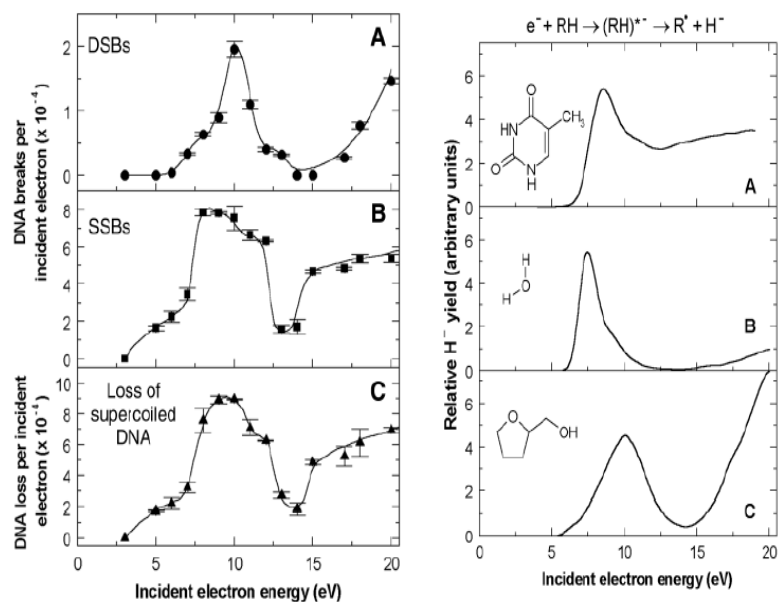
Science, **287** 1658 (2000)

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

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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

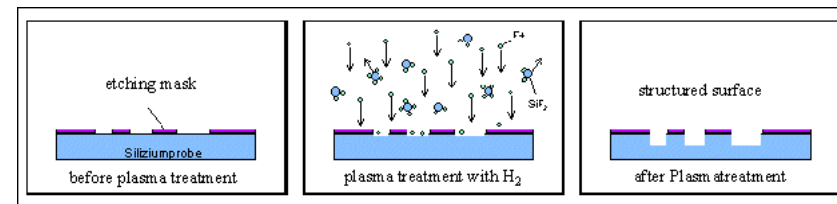# Surface treatment with Plasmas

Plasma Processing Gases ➡ Several Industry Applications

Production of reactive species ➡ ETCHING, DIAMANTIZATION, POLIMERIZATION, NITRIDING, CLEANING, and others

etching mask — Siliziumprobe — before plasma treatment

plasma treatment with H_2 — SiF$_2$ — F+

structured surface — after Plasm atreatment

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

Setting the problem

Elastic

THE COLLISION CAN BE

Inelastic

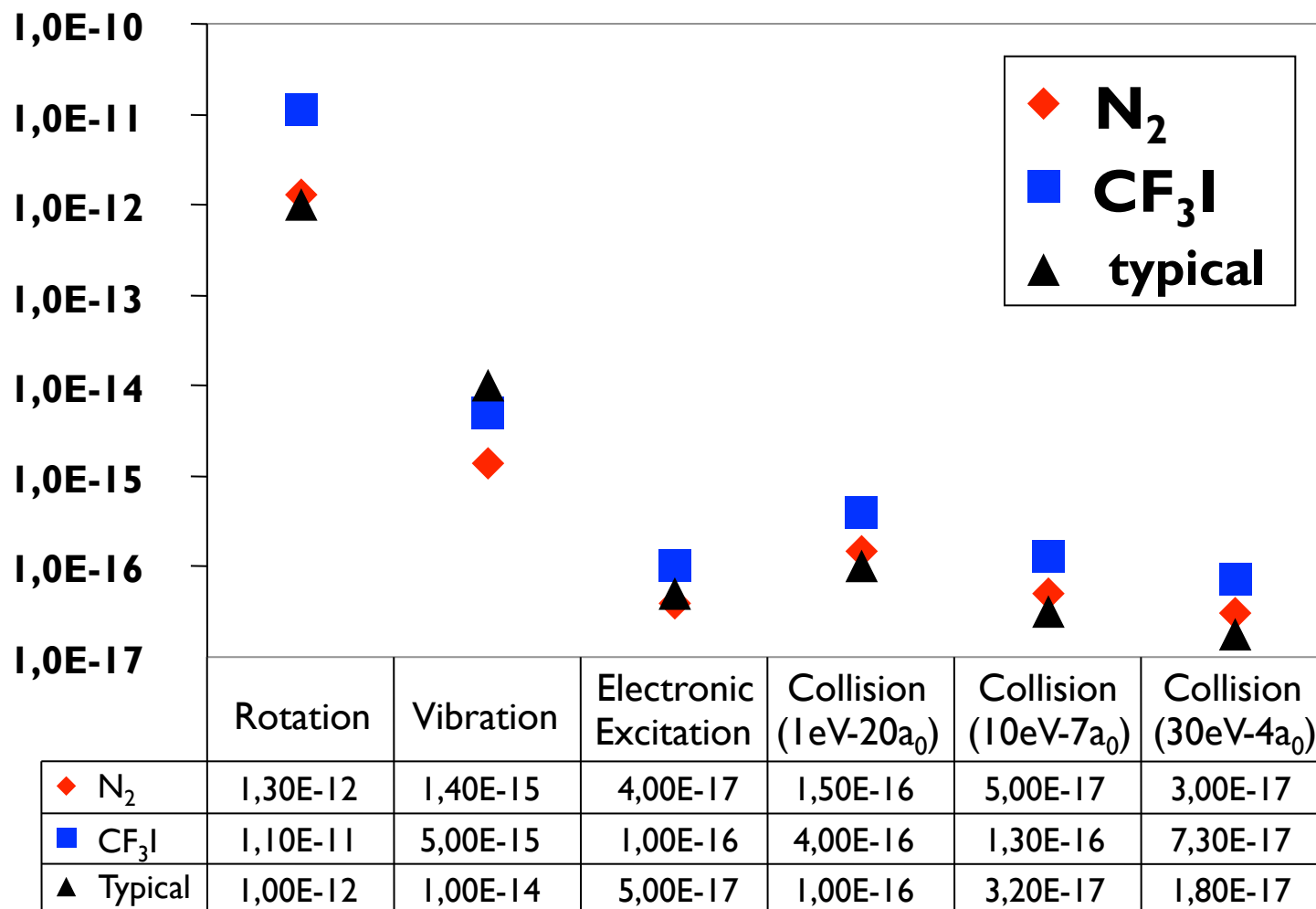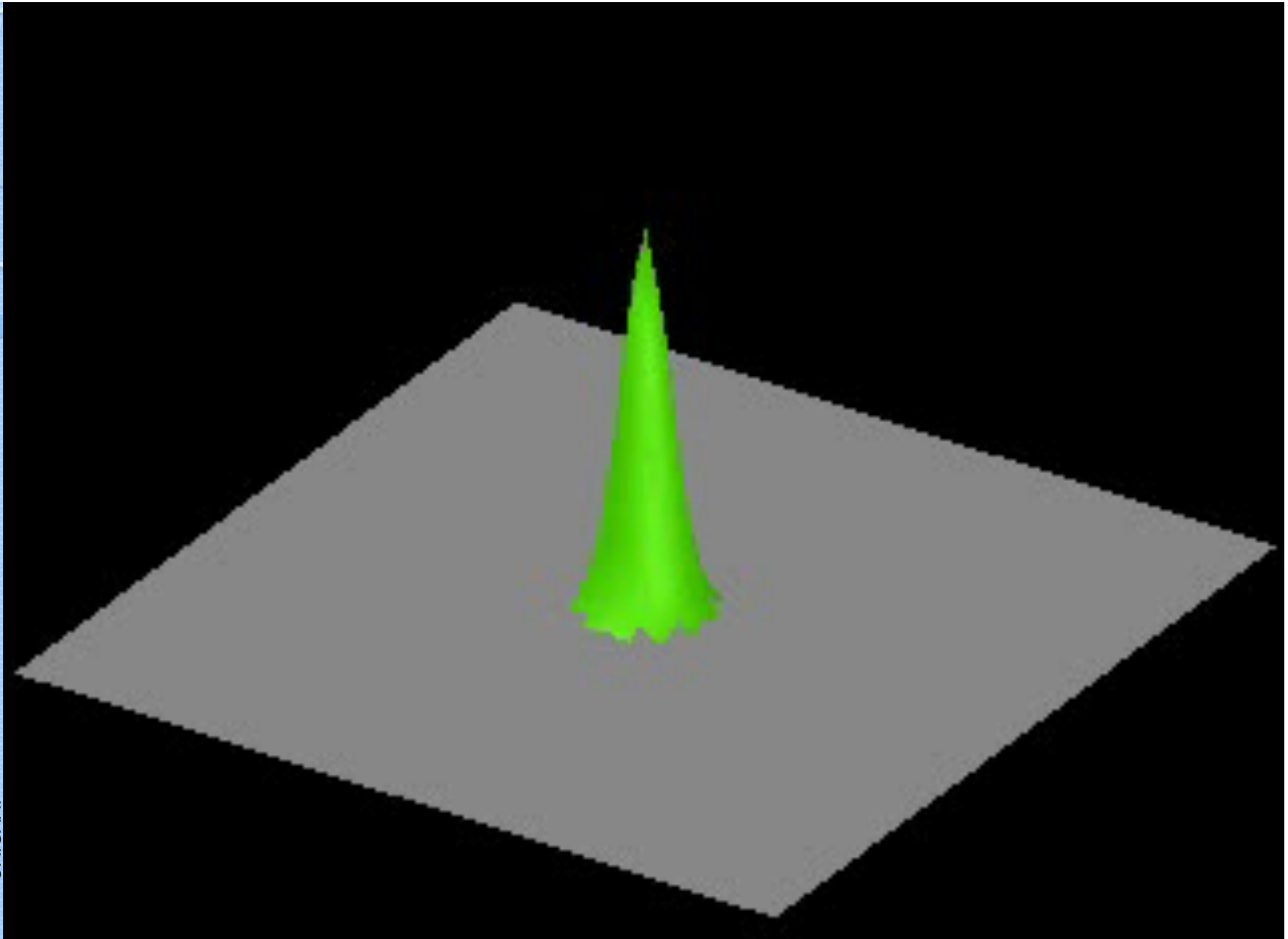| Excitation	Dissociation	Ionization
Rotational	Direct (vibrational excitation)	
Vibrational	Via electronic excitations	
Electronic	Via ressonance (with e without Attachment)	

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Setting the problem

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$_3$I	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

Legend:
- ◆ N$_2$
- ■ CF$_3$I
- ▲ typical
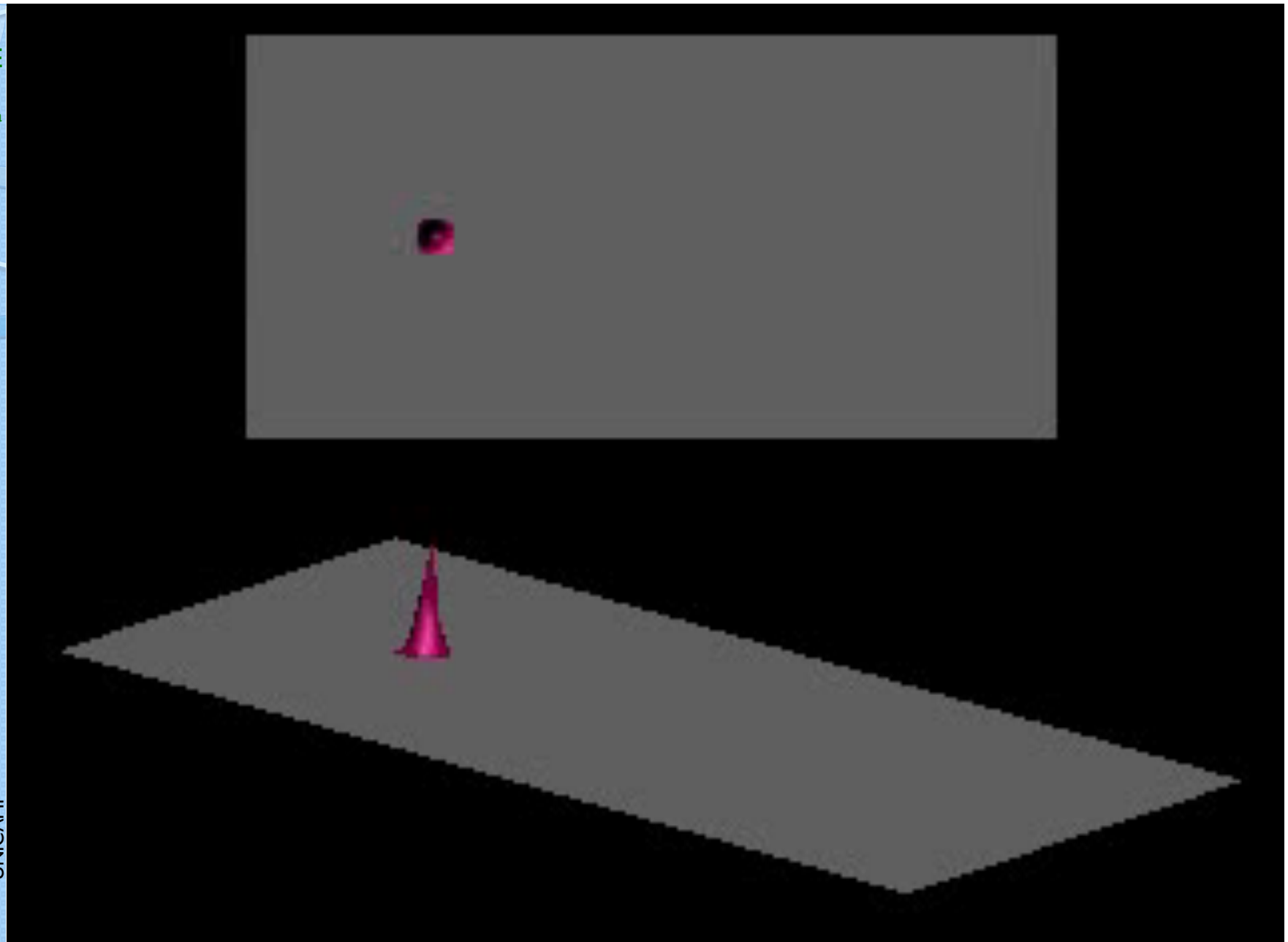
Partícula livre

Para ver as animações, visite: **http://www.embd.be/quantummechanics/**

Partícula prisioneira na caixa

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Para ver as animações, visite: **http://www.embd.be/quantummechanics/**
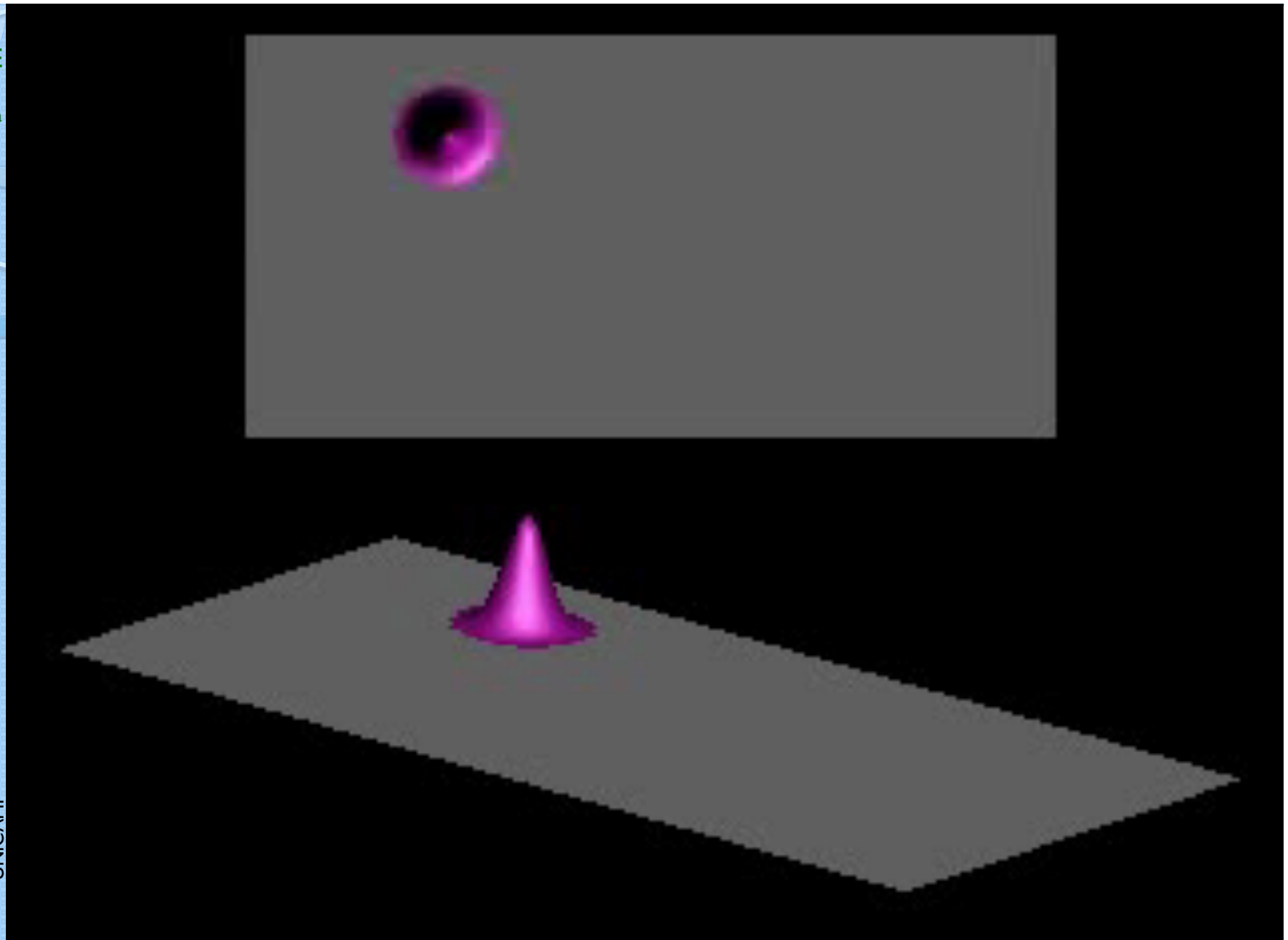
Partícula carregada em um campo magnético constante

Para ver as animações, visite: **http://www.embd.be/quantummechanics/**
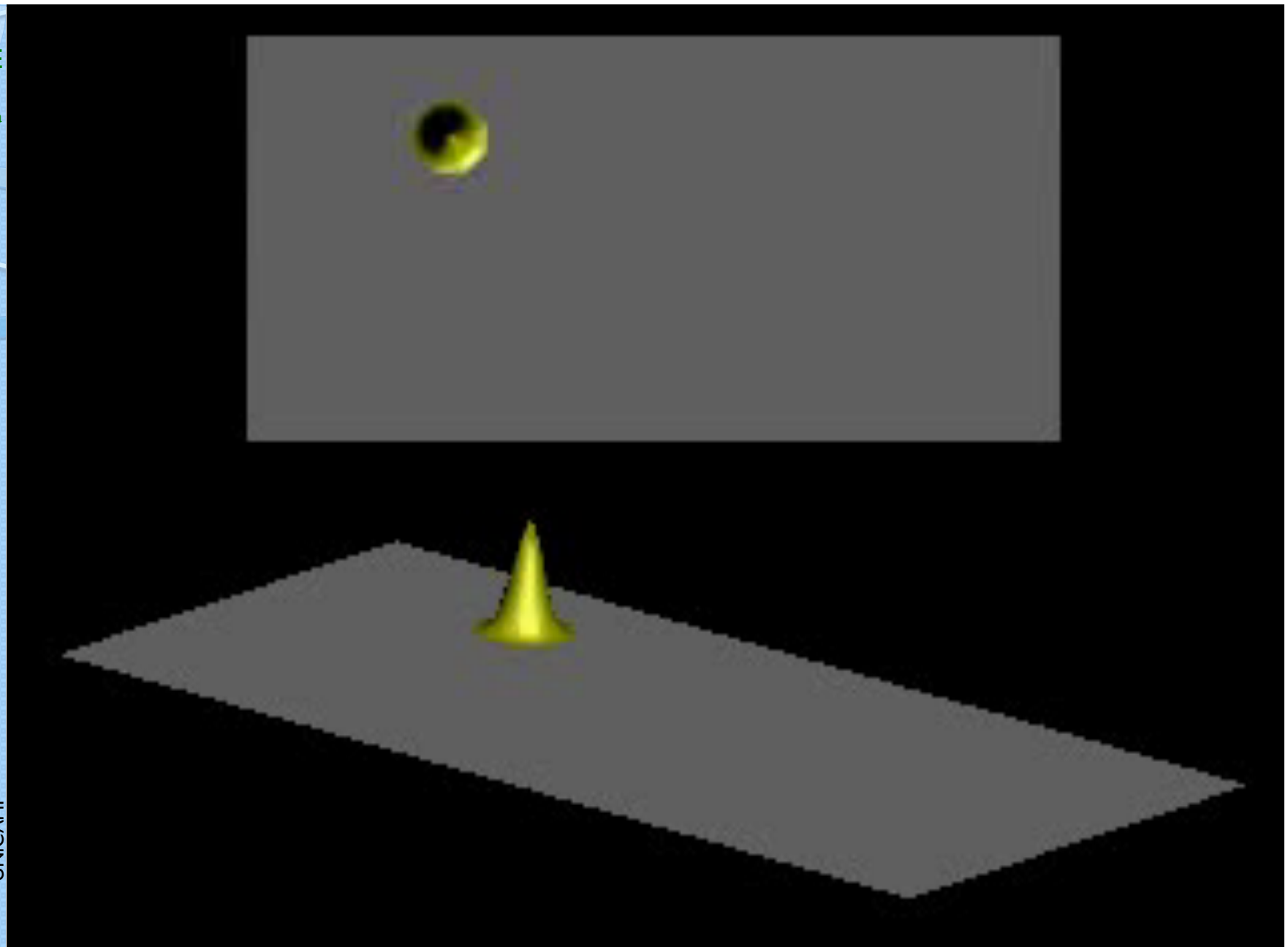
Partícula carregada na caixa em um campo magnético constante

Para ver as animações, visite: **http://www.embd.be/quantummechanics/**
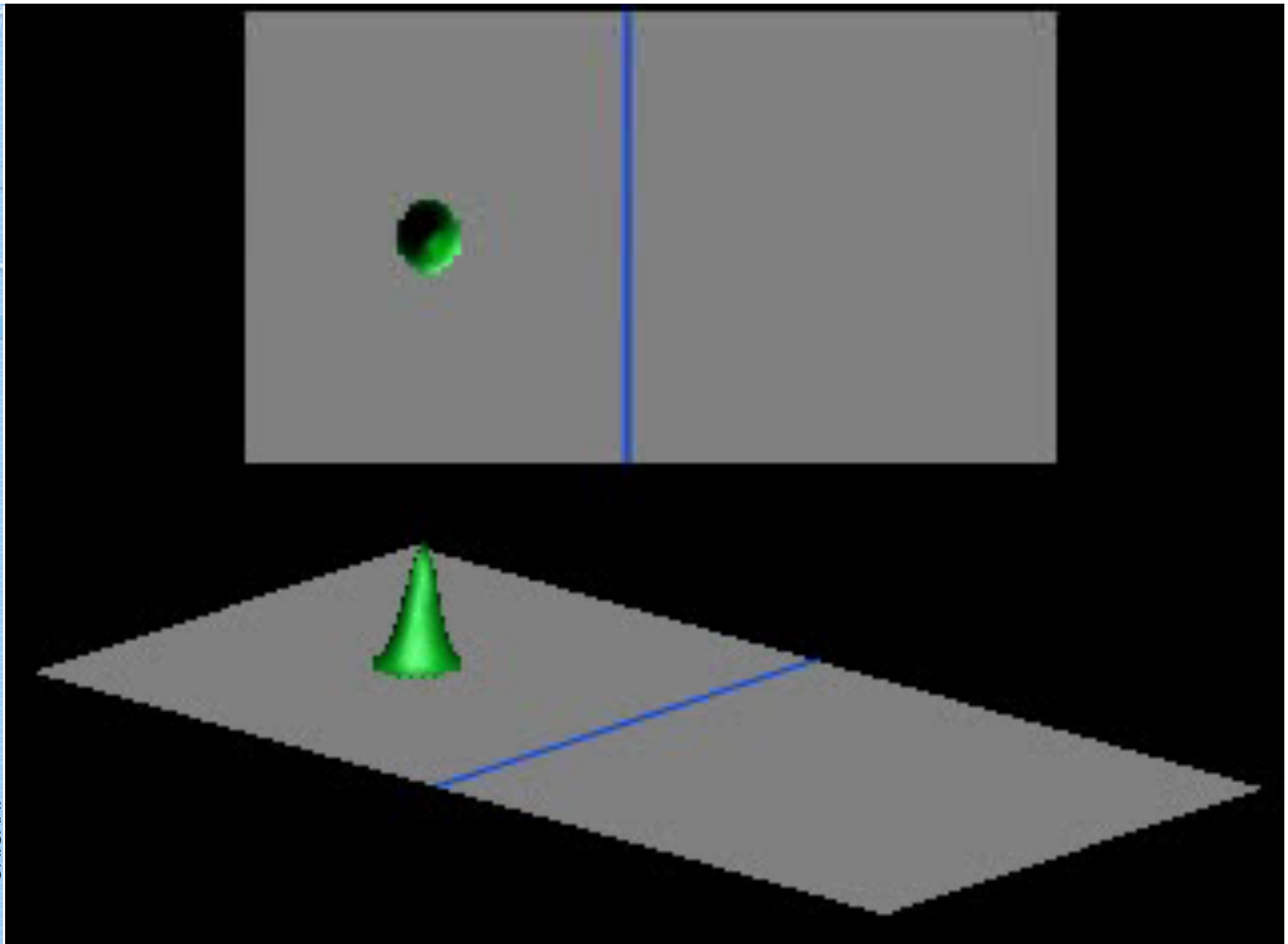
Efeito Túnel

Para ver as animações, visite: **http://www.embd.be/quantummechanics/**

Difração: uma fenda

MAPLima

Para ver as animações, visite: **http://www.embd.be/quantummechanics/**
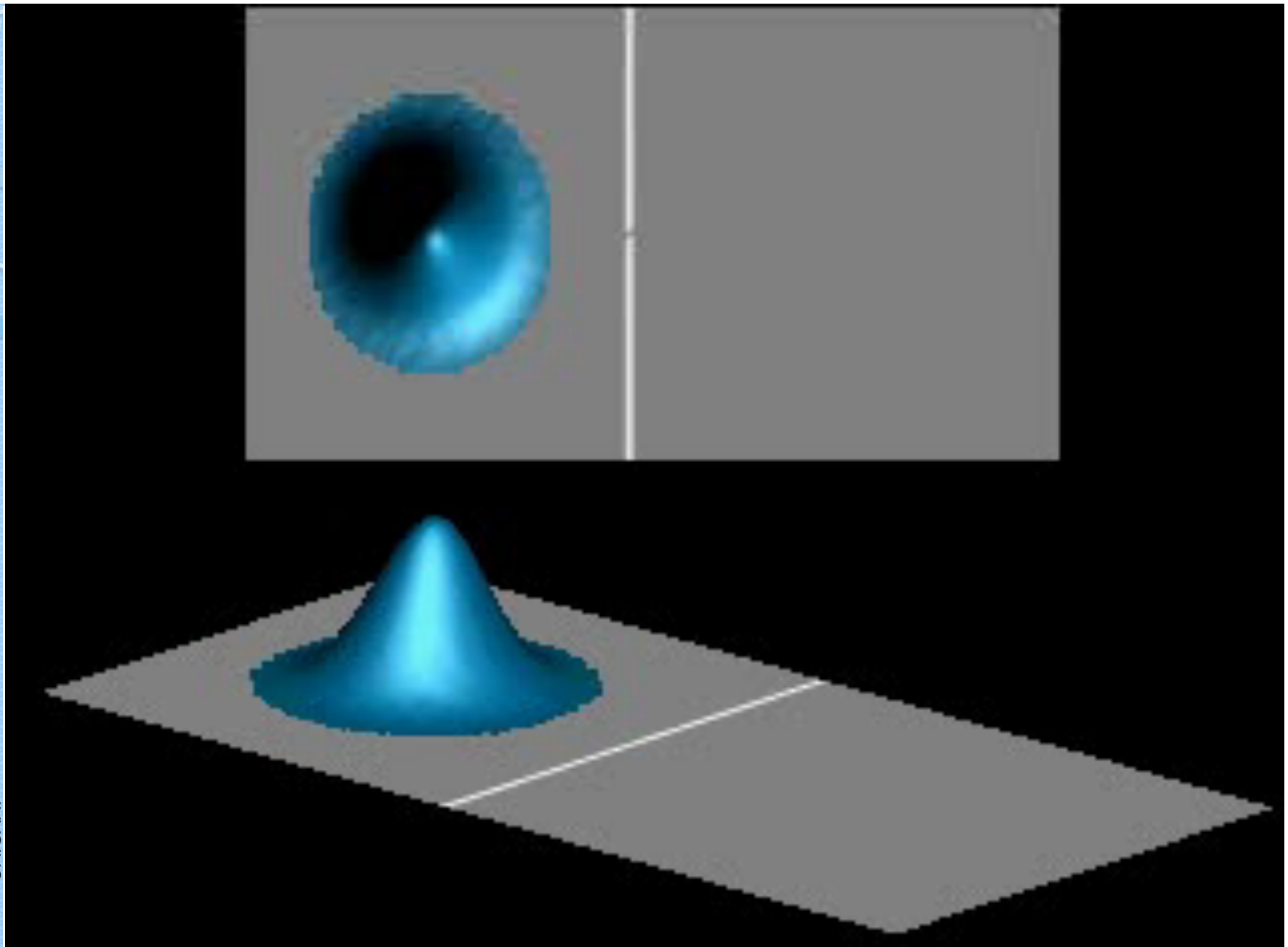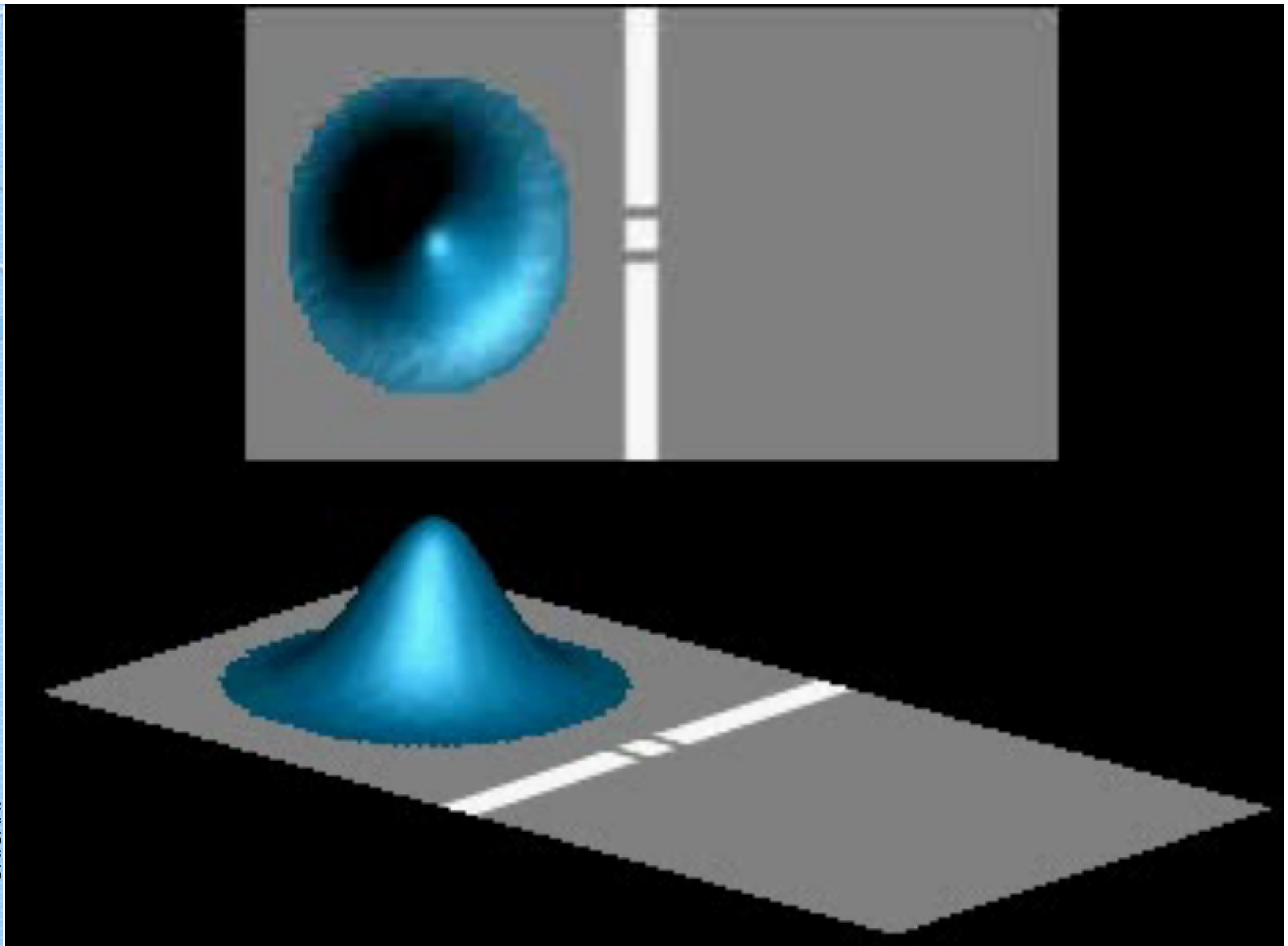
Interferência – duas fendas

Para ver as animações, visite: **http://www.embd.be/quantummechanics/**

Setting the problem

31

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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

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.*,

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

$$H_N \Phi_l = E_l \Phi_l$$ ➡ 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

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

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

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

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

Differential cross section

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

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

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

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

Free-particle Green's function

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

Theoretical background

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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:

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

Schwinger Variational Principle

Using Dirac´s notation:

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

where $\mid \Psi_{\vec{k}_i}^{(+)} \rangle$ satisfies:

$$\mid \Psi_{\vec{k}_i}^{(+)} \rangle = \mid \vec{k}_i \rangle + G_0^{(+)} V \mid \Psi_{\vec{k}_i}^{(+)} \rangle$$

Multiplying this expression by V, we have:

$$V \mid \Psi_{\vec{k}_i}^{(+)} \rangle = V \mid \vec{k}_i \rangle + V G_0^{(+)} V \mid \Psi_{\vec{k}_i}^{(+)} \rangle$$

$$A^{(+)} \mid \Psi_{\vec{k}_i}^{(+)} \rangle = V \mid \vec{k}_i \rangle$$

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

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

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

where:

$$A^{(-)} = V - V G_0^{(-)} V$$

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

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Schwinger Variational Principle

So, our problem is to solve the equations:

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

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

Theoretical background

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

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

39

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Skip it

Schwinger Variational Principle

Theoretical background

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

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XI WFME
2013
Feira de Santana

Theoretical background

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41

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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:
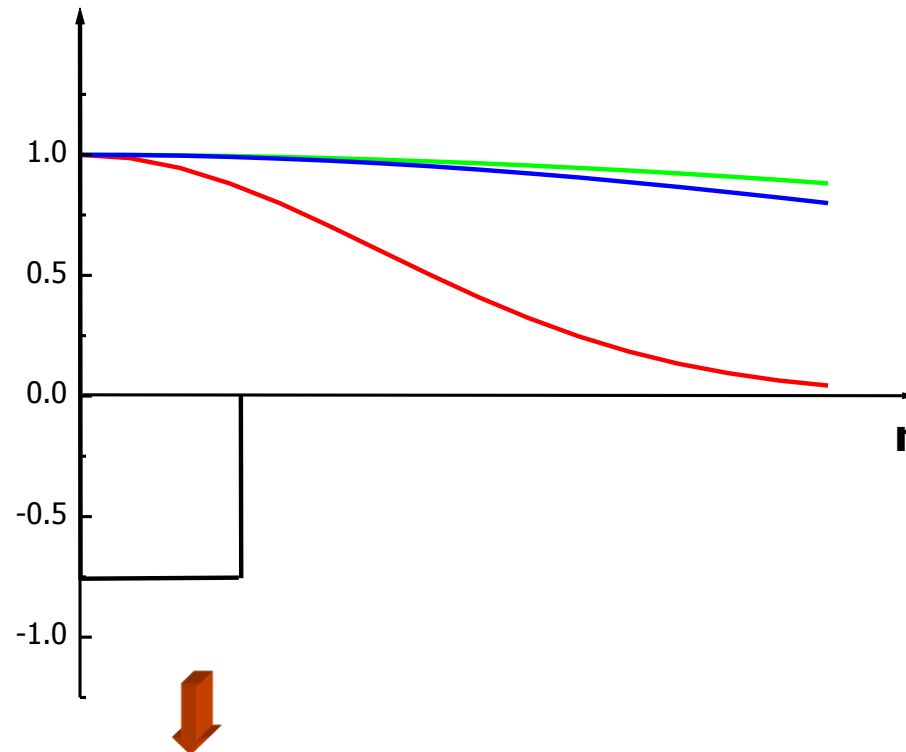
gives rise to spurious structures of
numerical nature

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

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

Skip it

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

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42

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

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43

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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, $j \geq 2$ 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

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Coupling level

➡ Inelastic scattering with and without polarization

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

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

➡ $|\Phi_\ell\rangle$ 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

46

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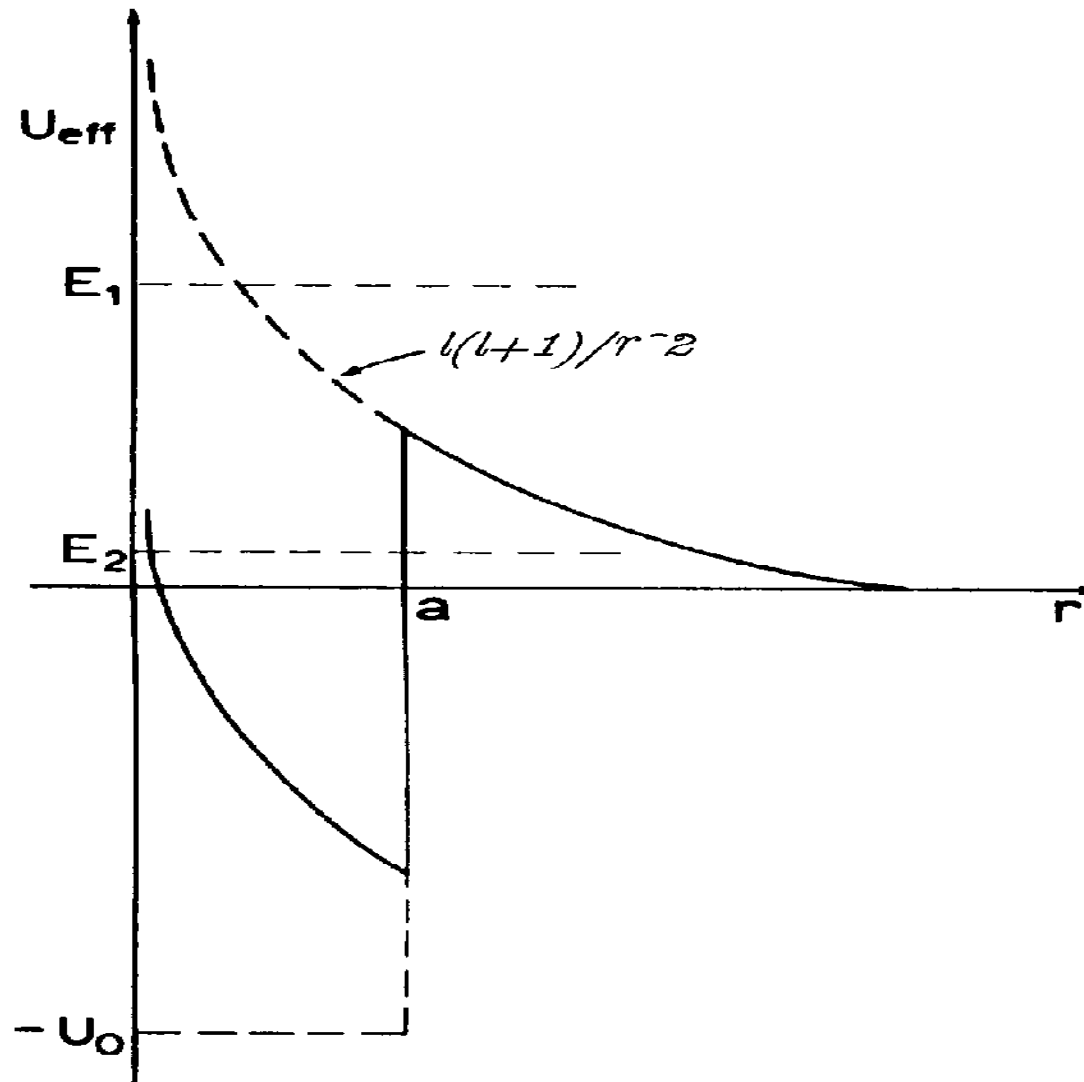
Low energy elastic electron scattering from pirrole

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

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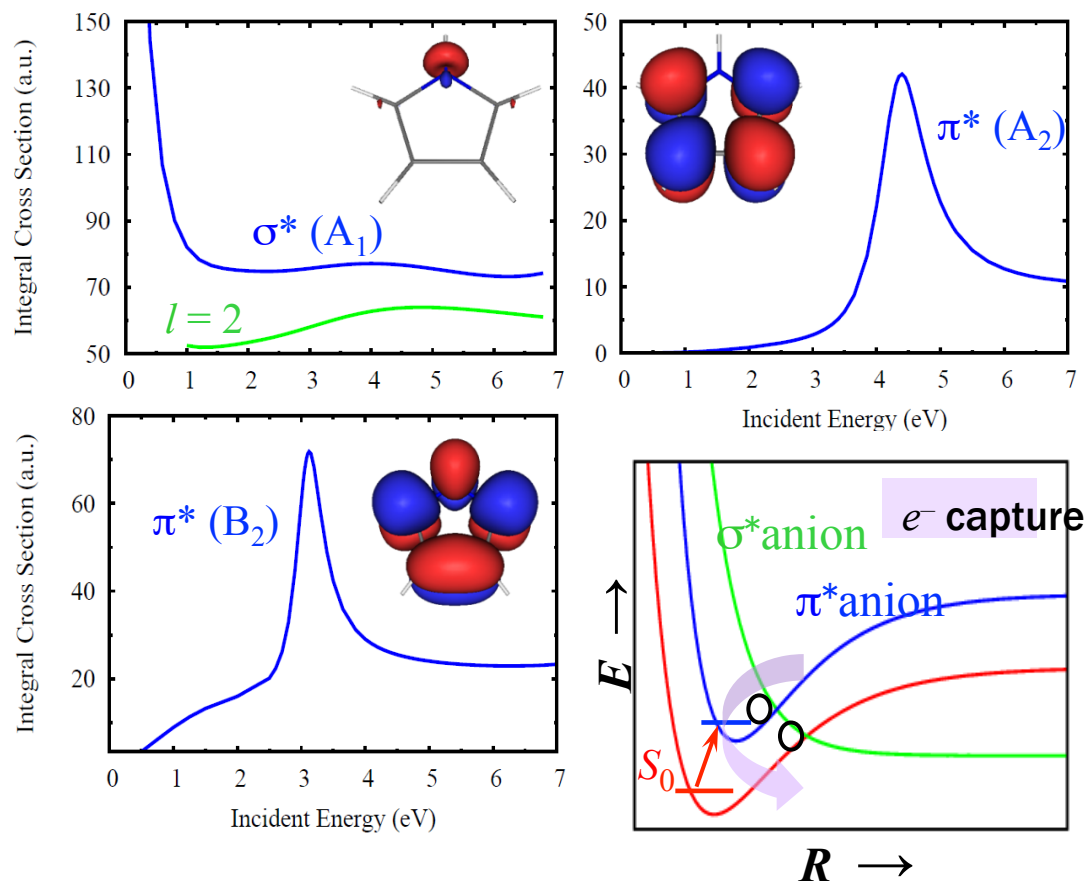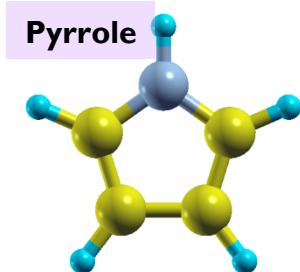
de Oliveira EM, Lima MAP, Bettega MHF, Sanchez SD, da Costa RF, and Varella MTD, J. Chem. Phys. **132**, 204301 (2010)

Lignin Subunits

Phenol

Guaiacol
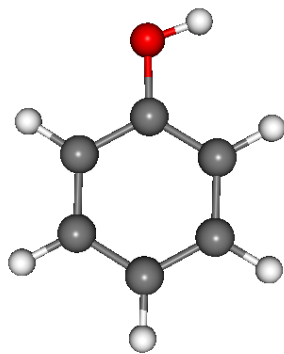
Syringol

MetOH
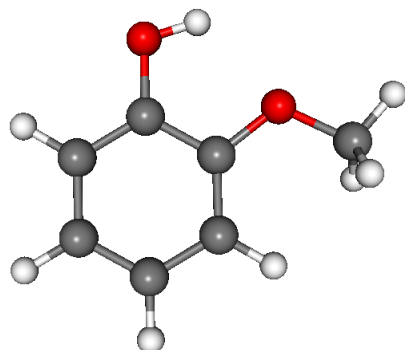
MetOH

PropenylOH
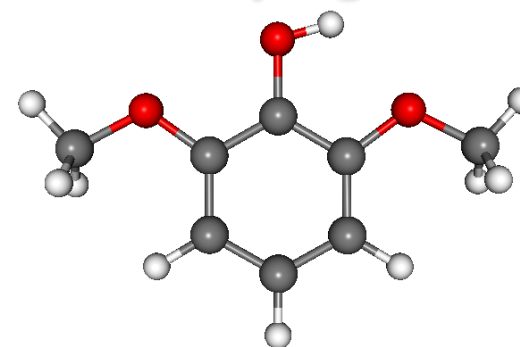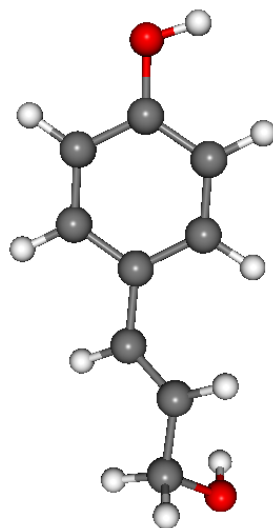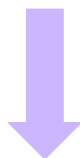
PropenylOH

PropenylOH

p-coumaryl alcohol
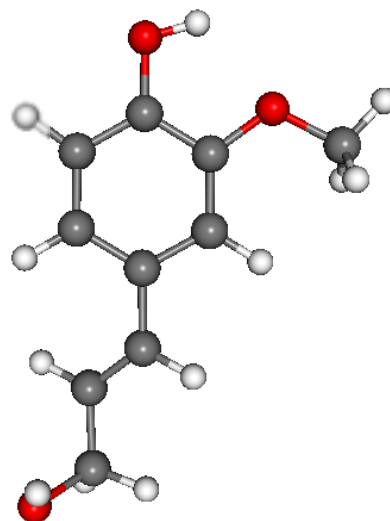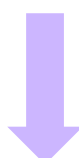
coniferyl alcohol

sinapyl alcohol

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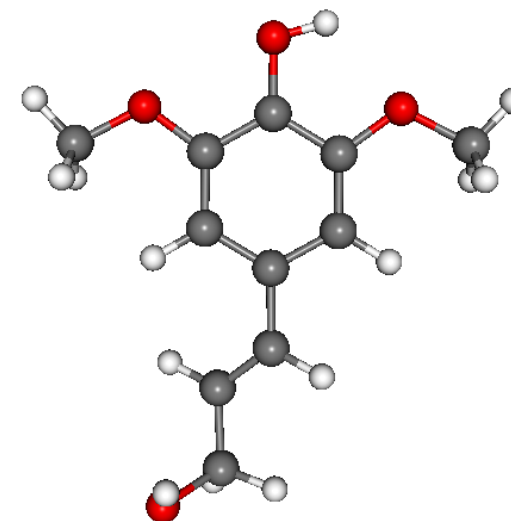
Shape resonance spectra of lignin subunits
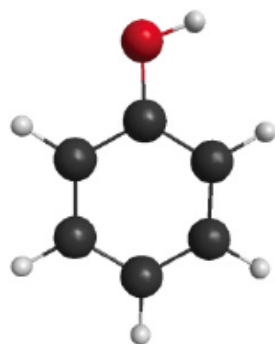
phenol

—— SEP

- - - SE

guaiacol

—— SEP

- - - SE

- - - SE

p-coumaryl alcohol

p-Cu (LUMO)

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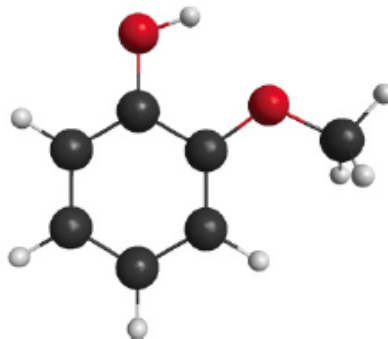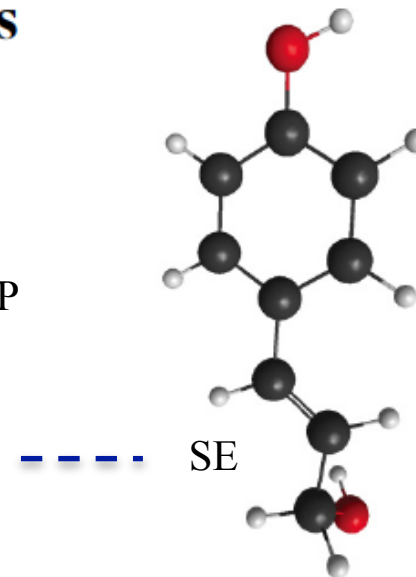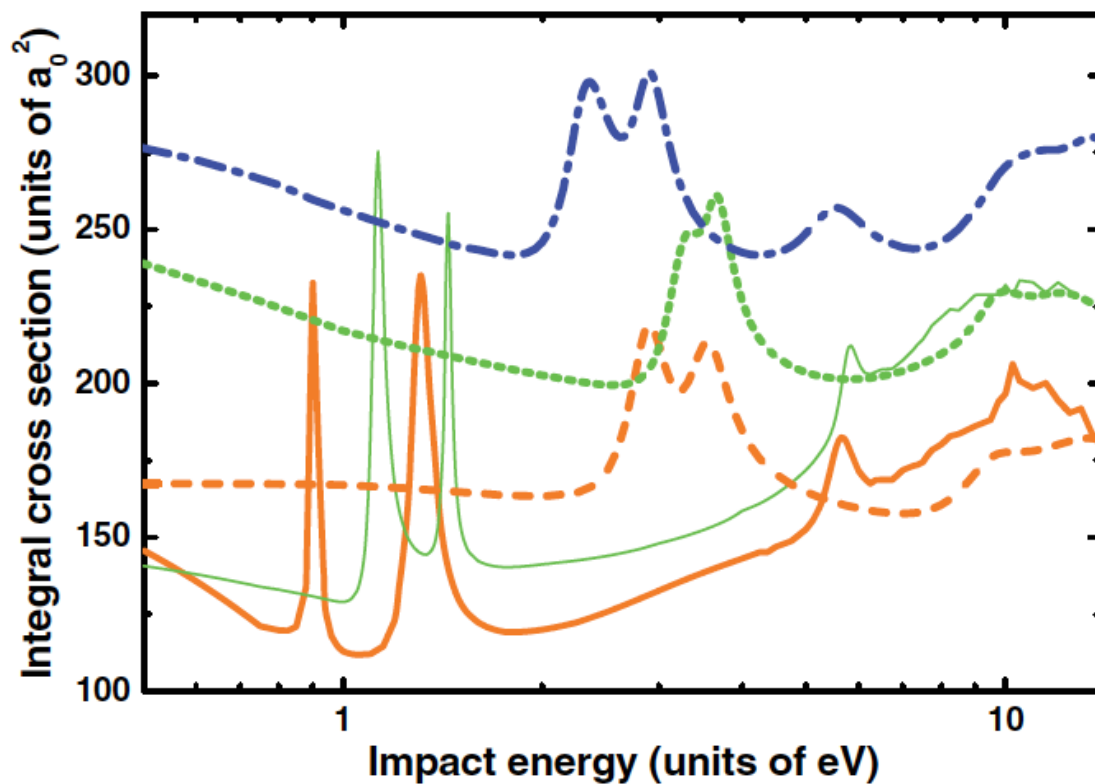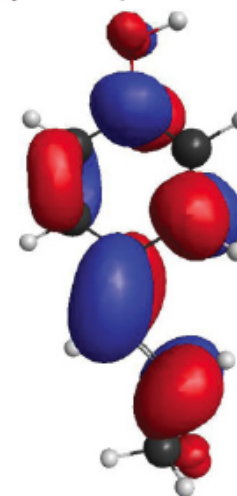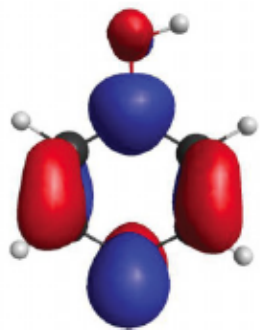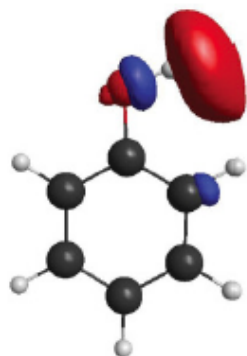
π* (LUMO+1)   σ* (LUMO+2)

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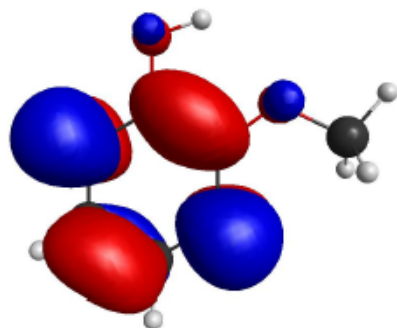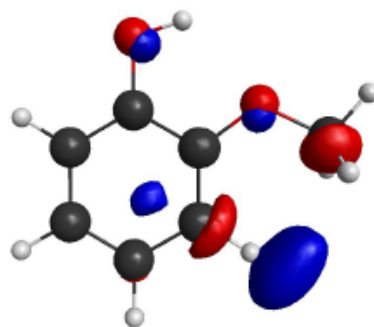
Guaiacol: Methoxilation is expected to give rise to other dissociation channels. H elimination should be also observed.

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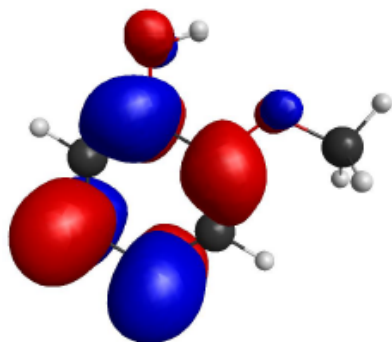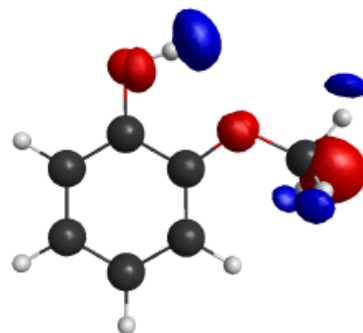
Low-energy electron scattering by cellulose and Hemicellulose components

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

(a) β-D-glucose

(b) α-D-glucose

(c) β-D-xylose

(d) cellobiose

(e) maltose

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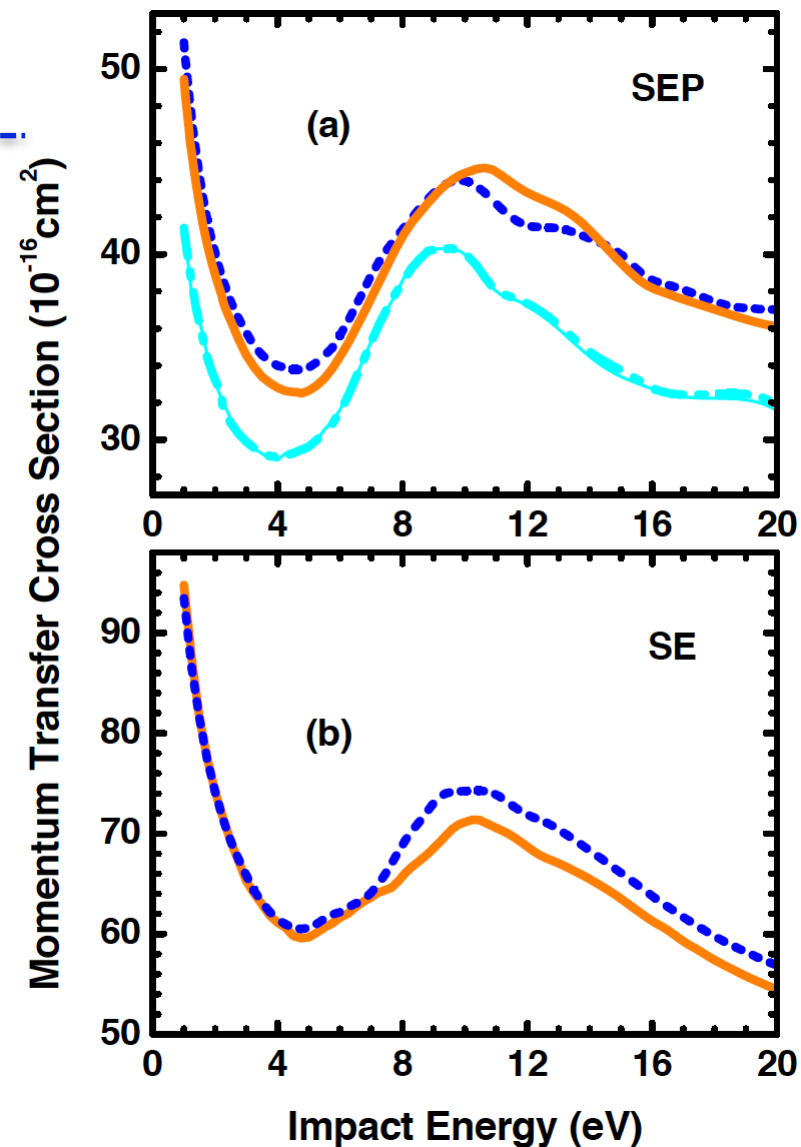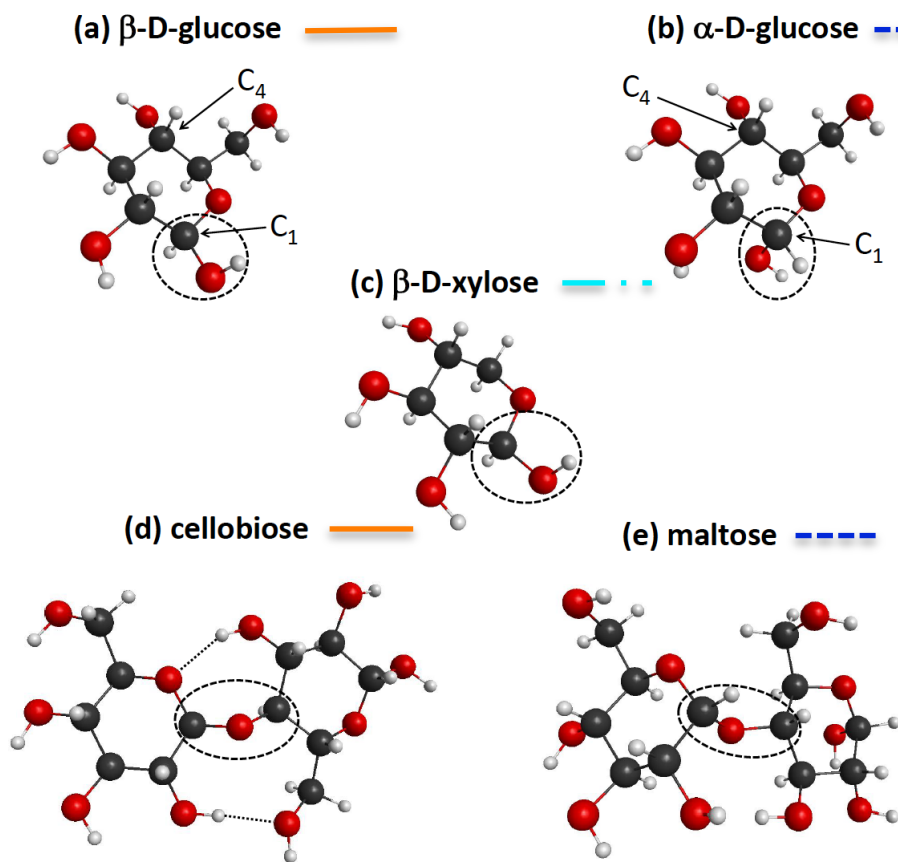
Theoretical team on electron-scattering of microsolvated molecules

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

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

UFPR
UNIVERSIDADE FEDERAL DO PARANÁ

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

Electron Collisions with the CH$_2$O-H$_2$O complex

PHYSICAL REVIEW A 80, 062710 (2009)
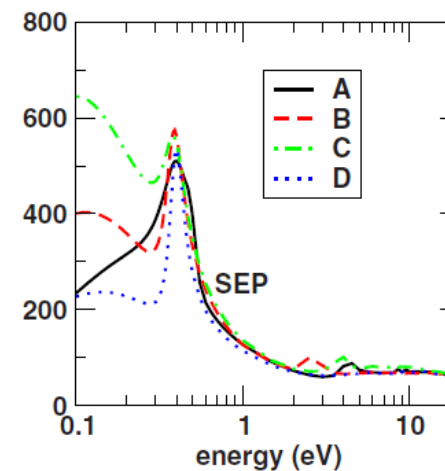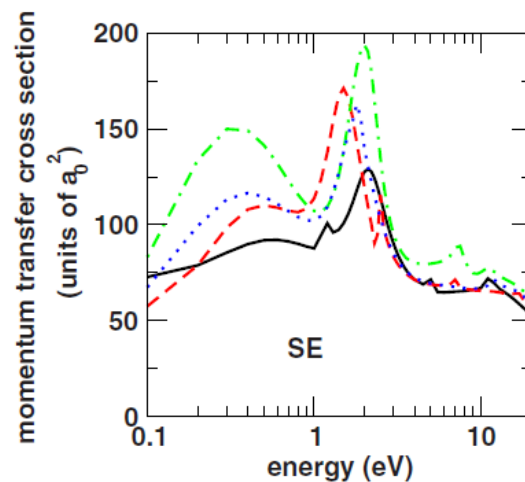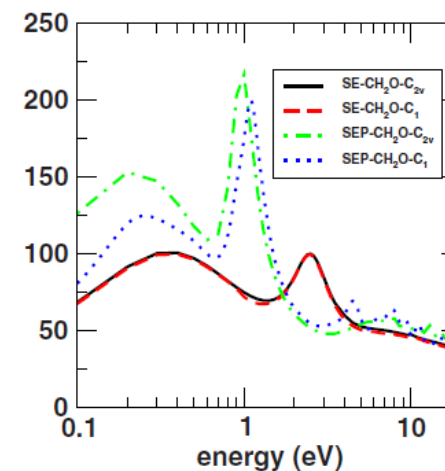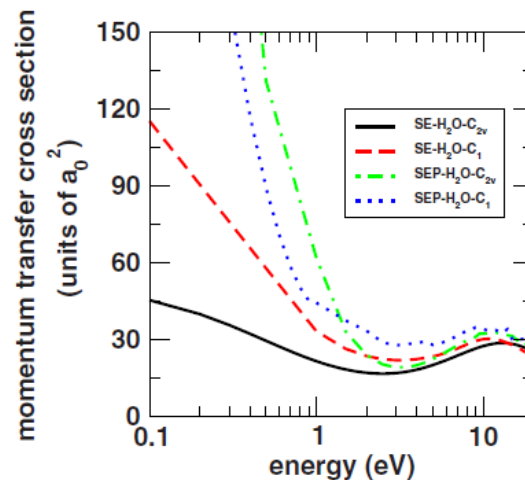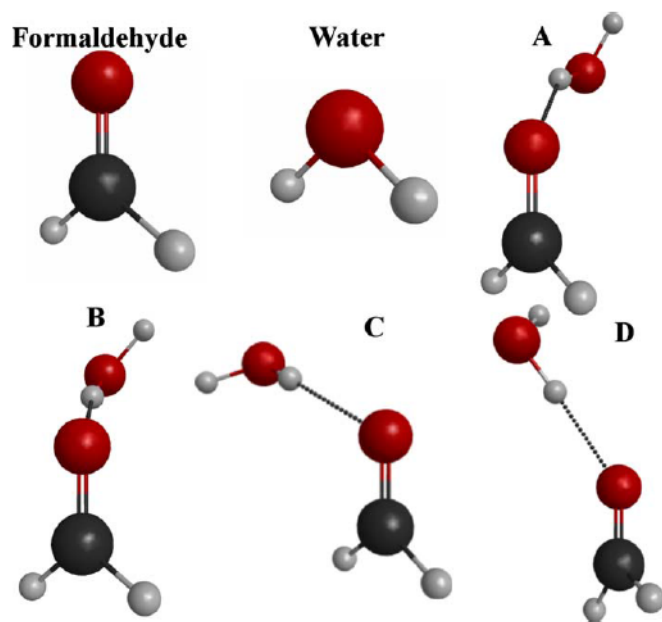
Electron collisions with the HCOOH…(H₂O)n complexes (n=1, 2) in liquid phase: The influence of microsolvation on the π* resonance of formic acid

THE JOURNAL OF CHEMICAL PHYSICS **138**, 174307 (2013)
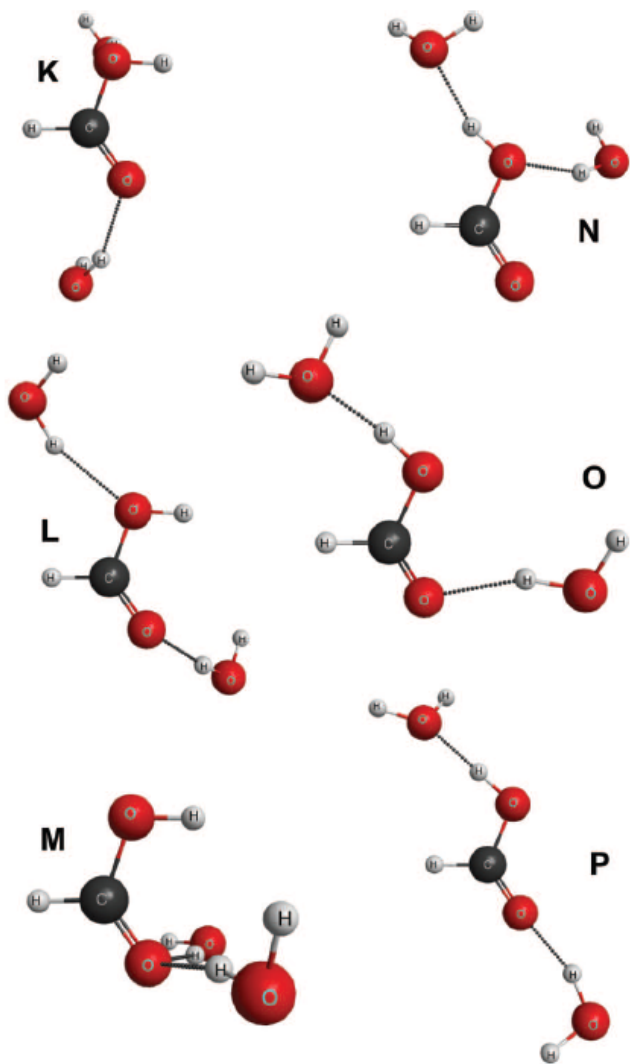
π^* shape resonance for HCOOH at around 1.9 eV.
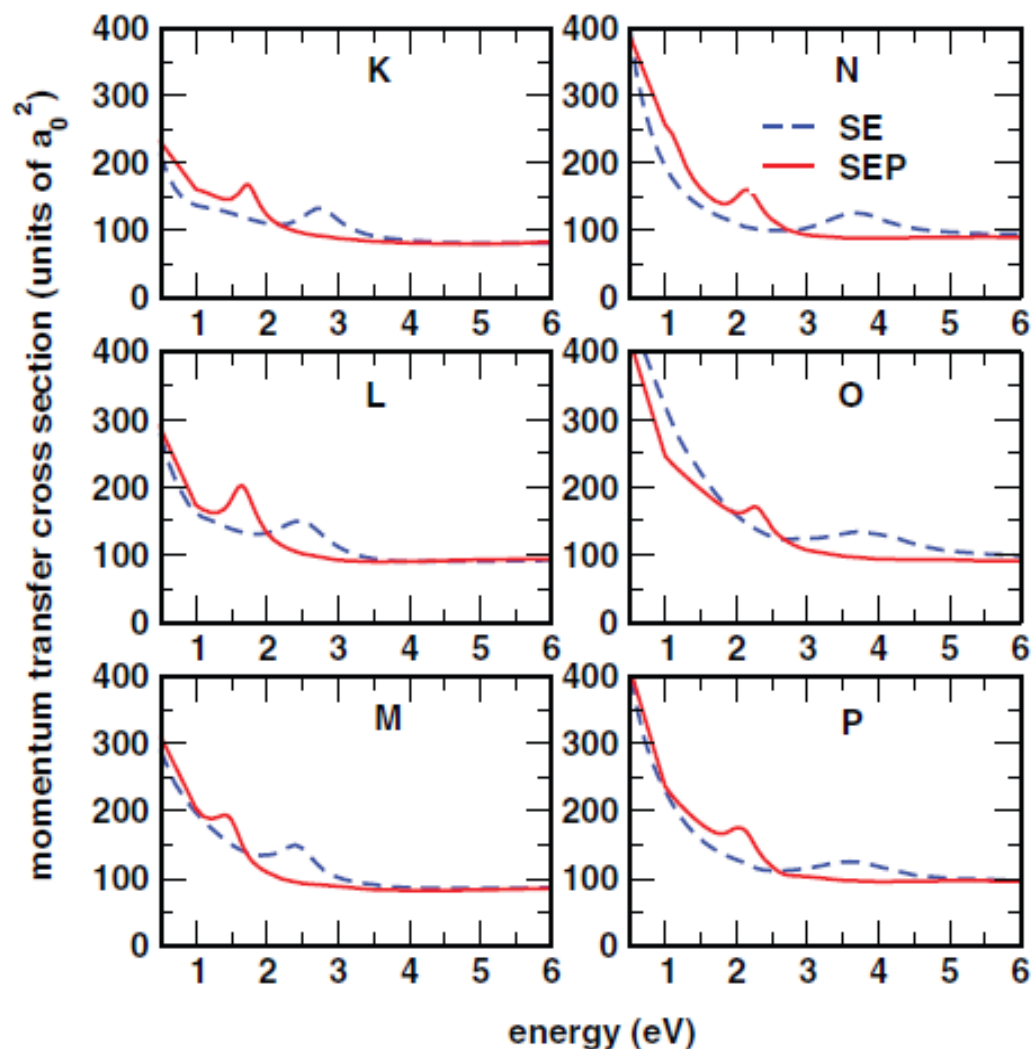
Electron Collisions with Phenol...H₂O: search for microsolvation signatures in the DCS
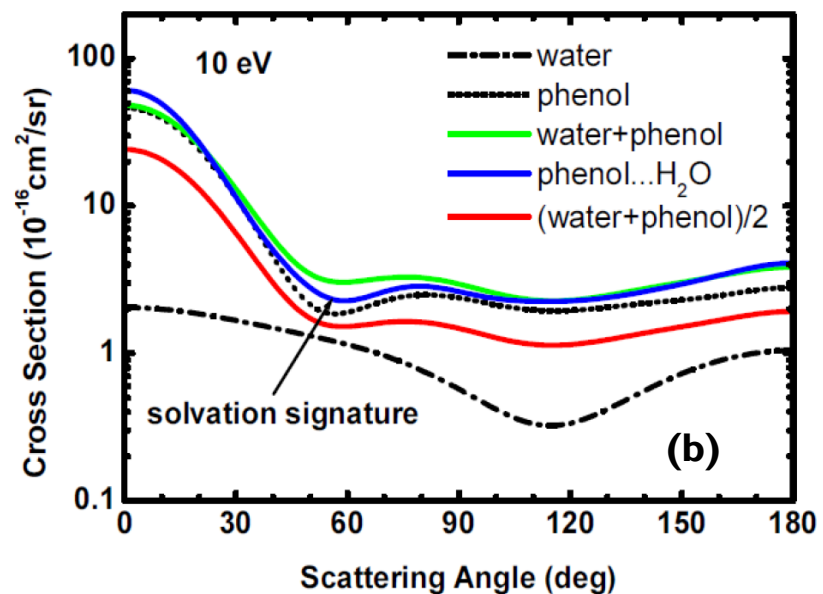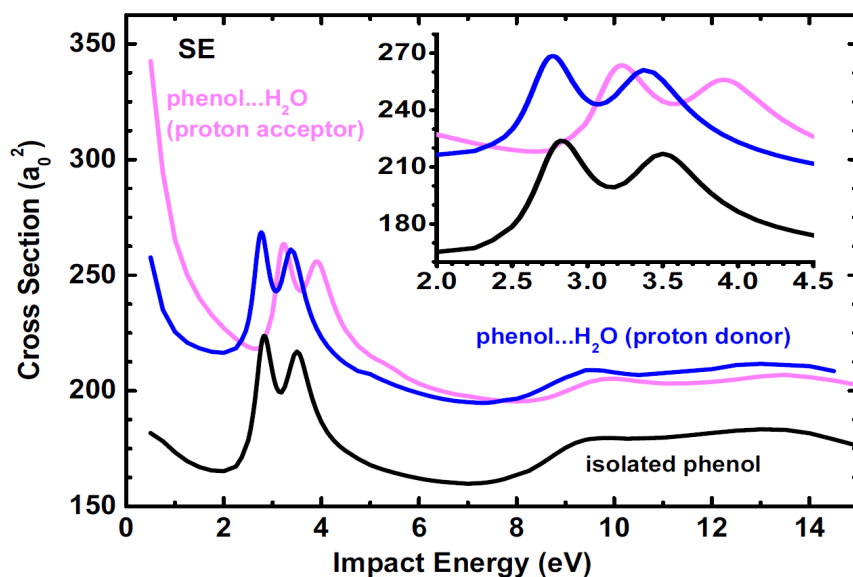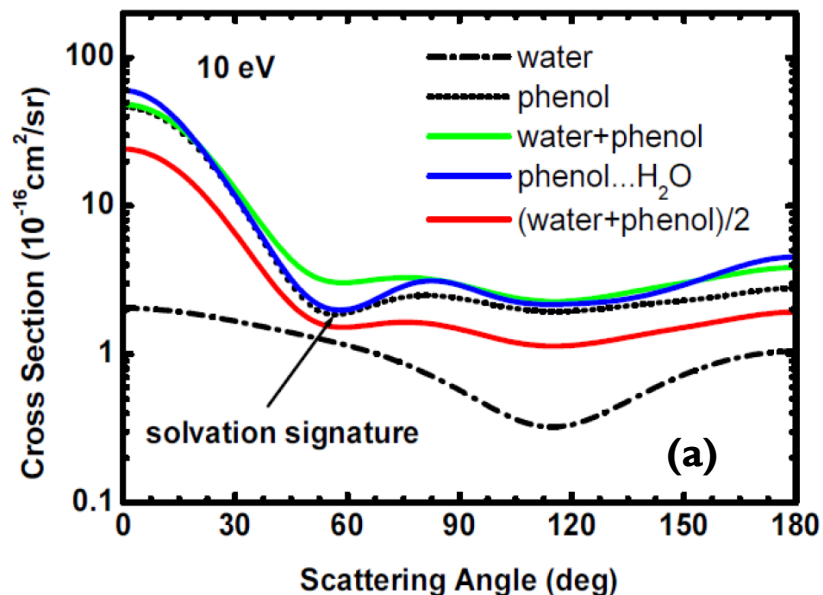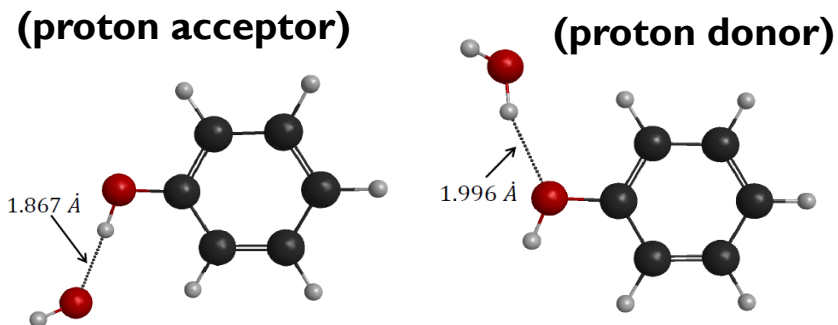
Electron Collisions with Phenol...(H$_2$O)$_2$: search for microsolvation signatures in the DCS

Static-Exchange Calculations:
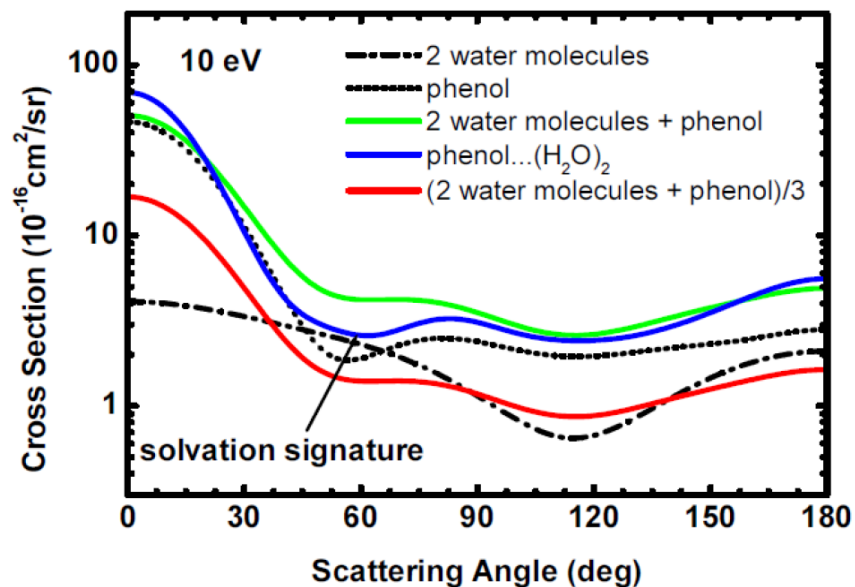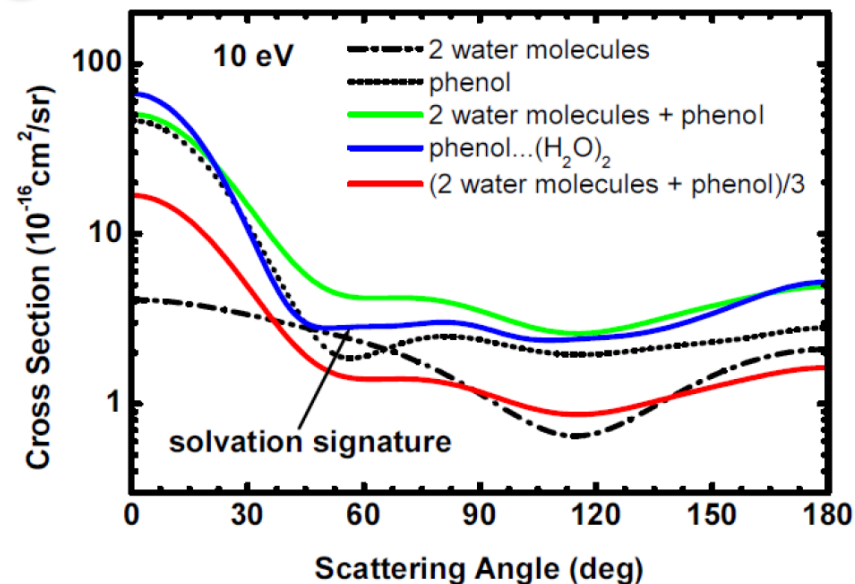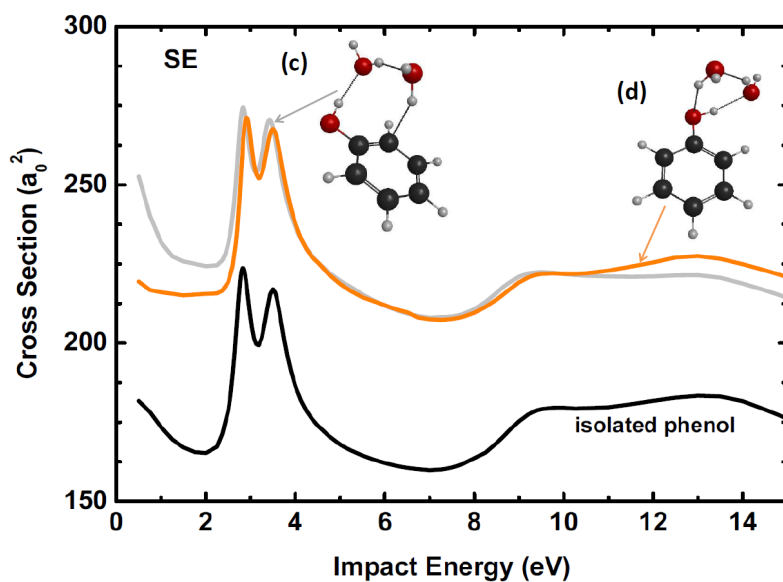
Electron Collisions with Phenol...(H$_2$O)$_n$: search for microsolvation signatures in the DCS

Static-Exchange Calculations:
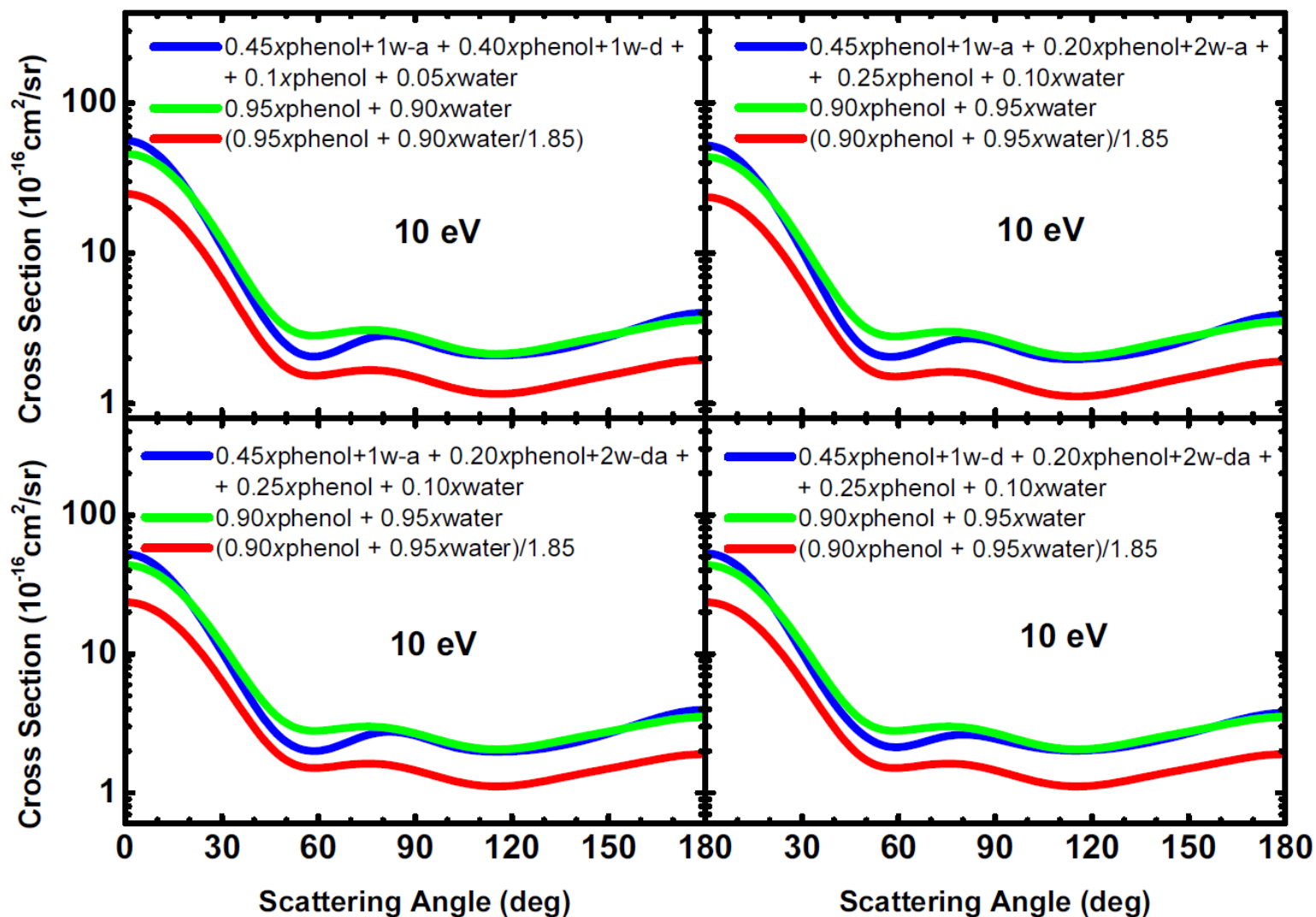
Electron Scattering of slow electrons by furfural molecules
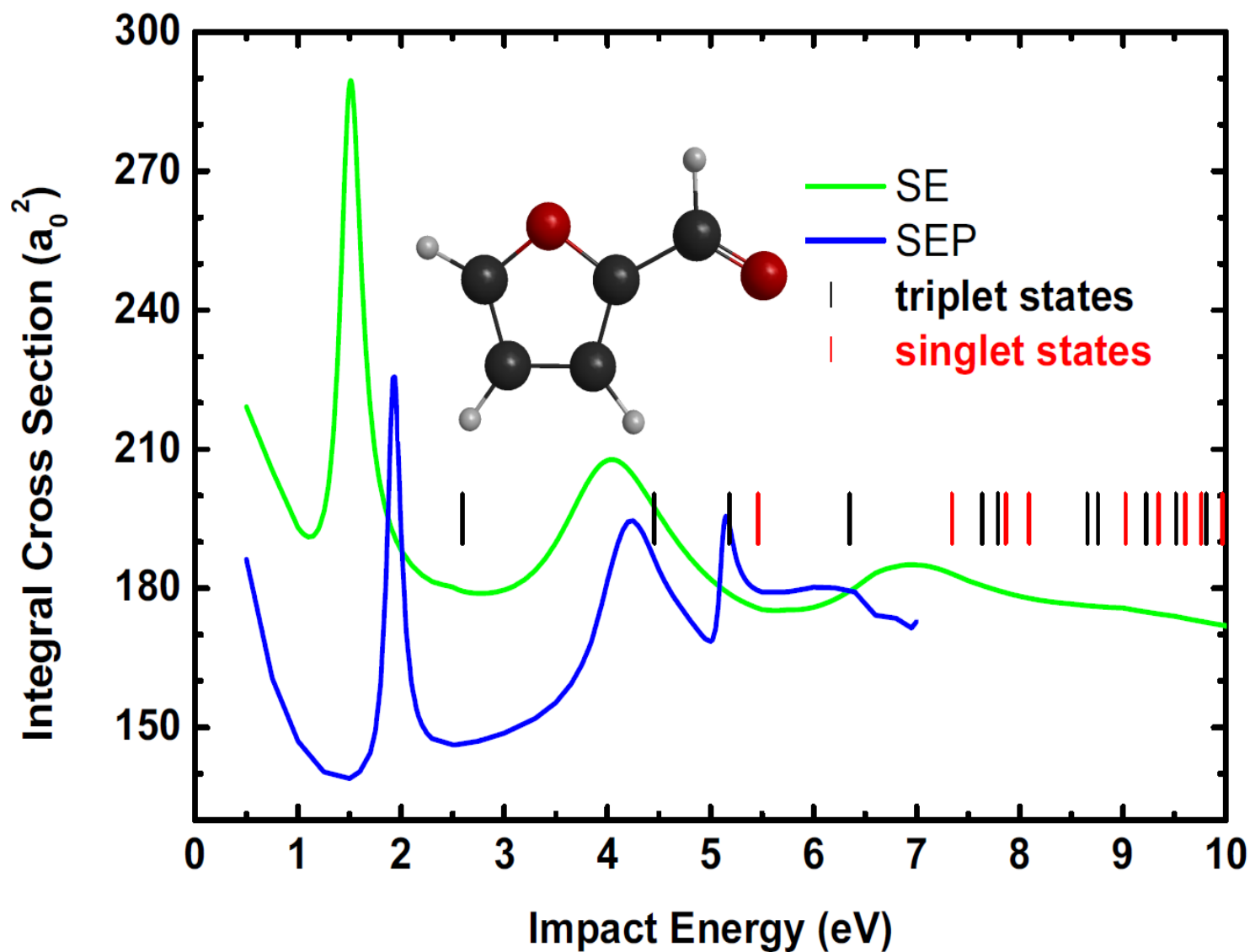
This molecule has over 20 electronic states between 0 and 10 eV

ELECTRONIC EXCITATION

Electronic excitation of H₂ by electron impact

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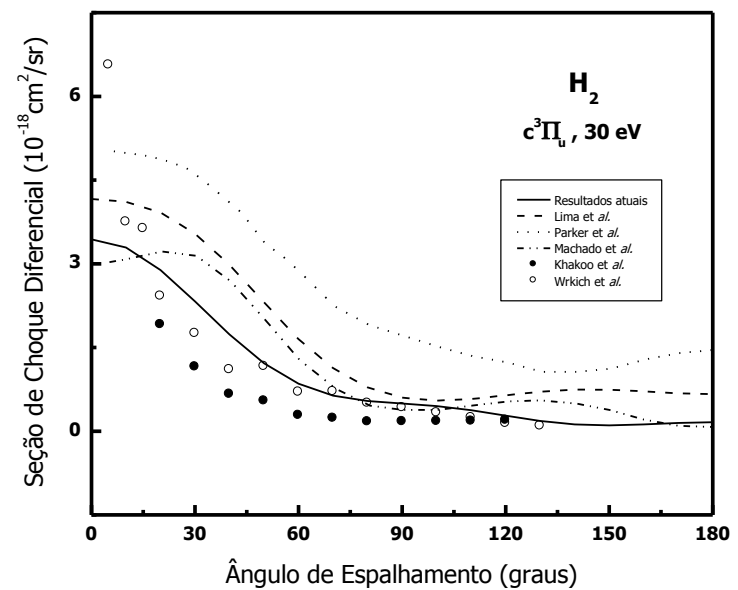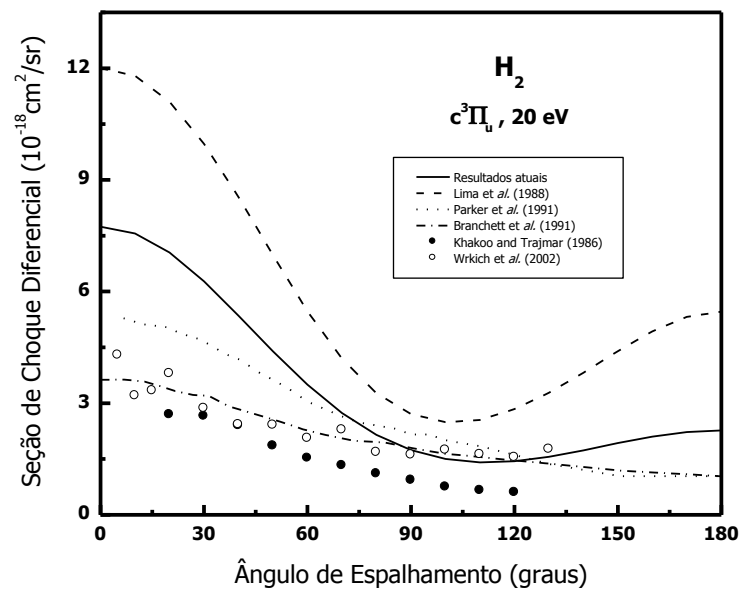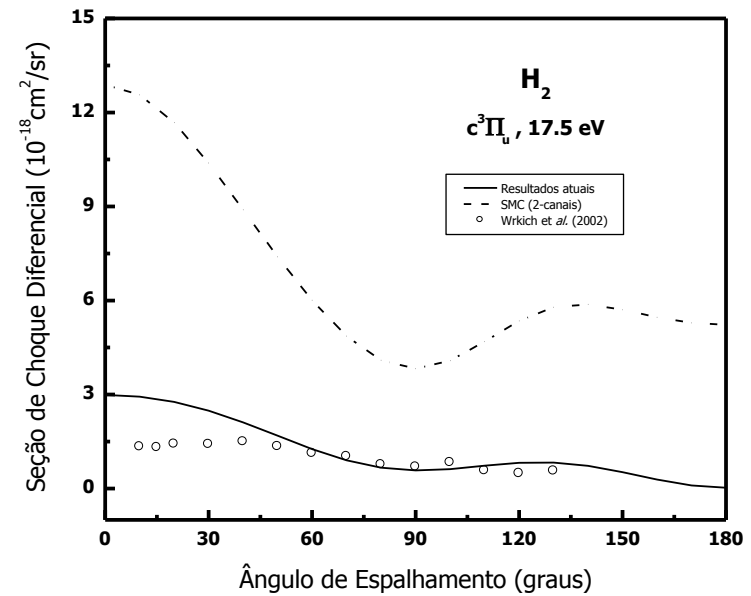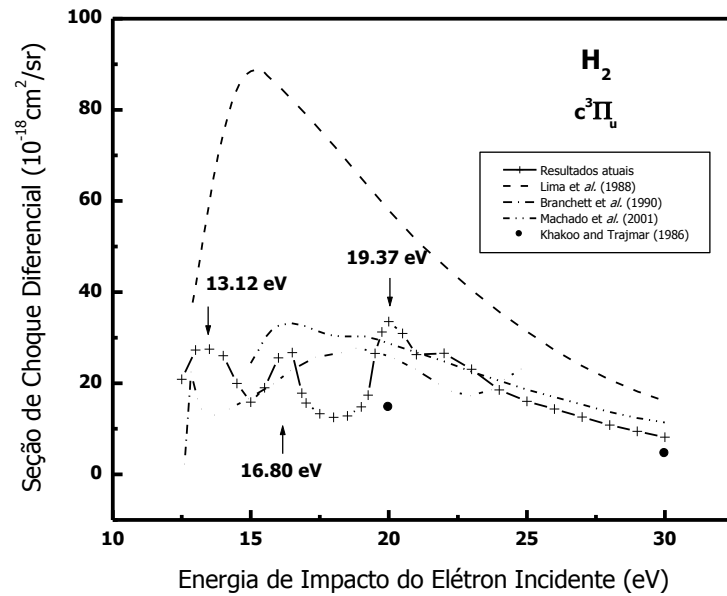
Electronic transition $X\ ^1\Sigma_g \rightarrow A\ ^3\Sigma_u^+$ of N_2 by electron impact
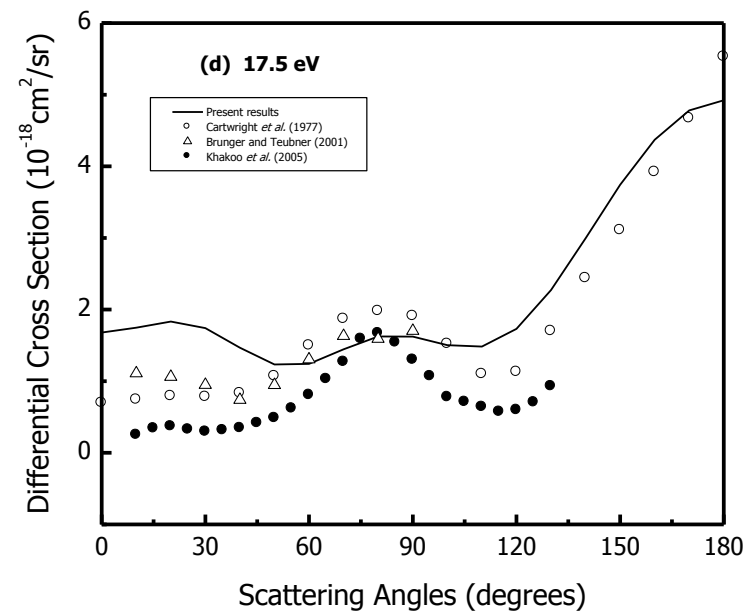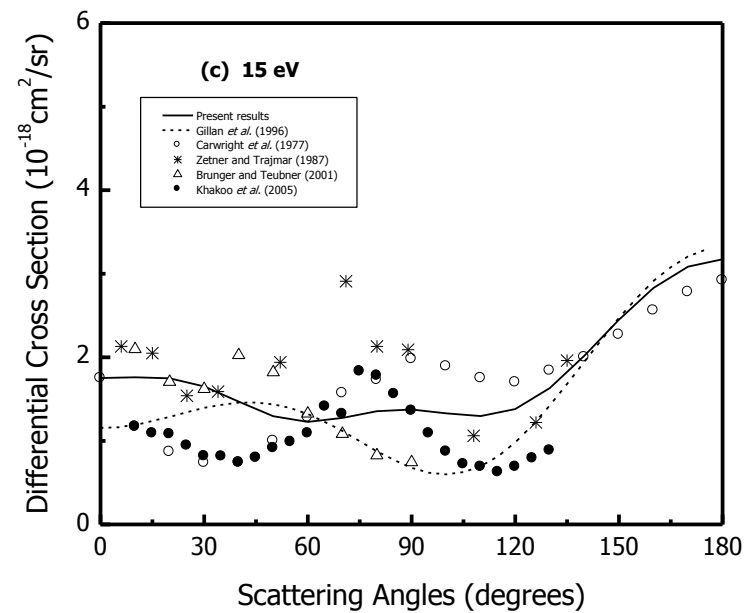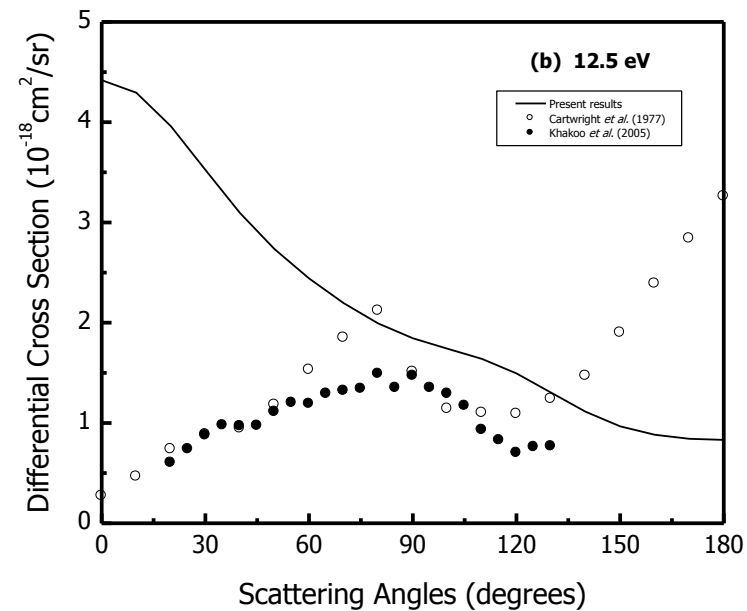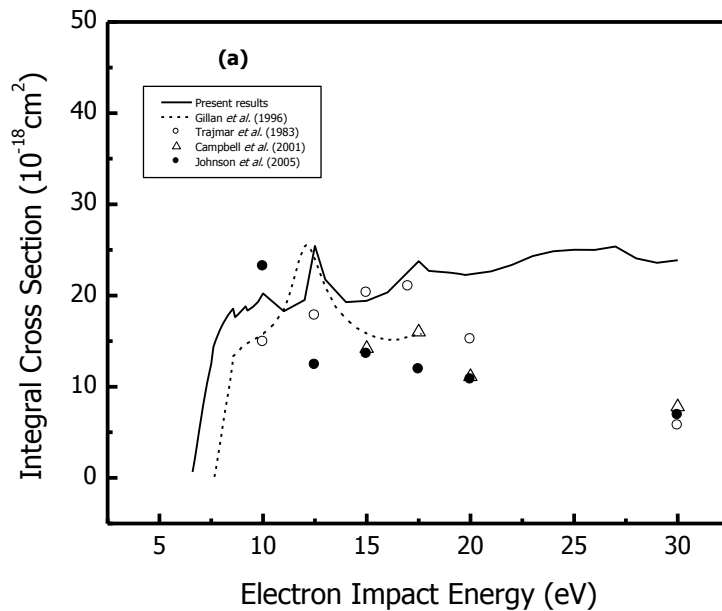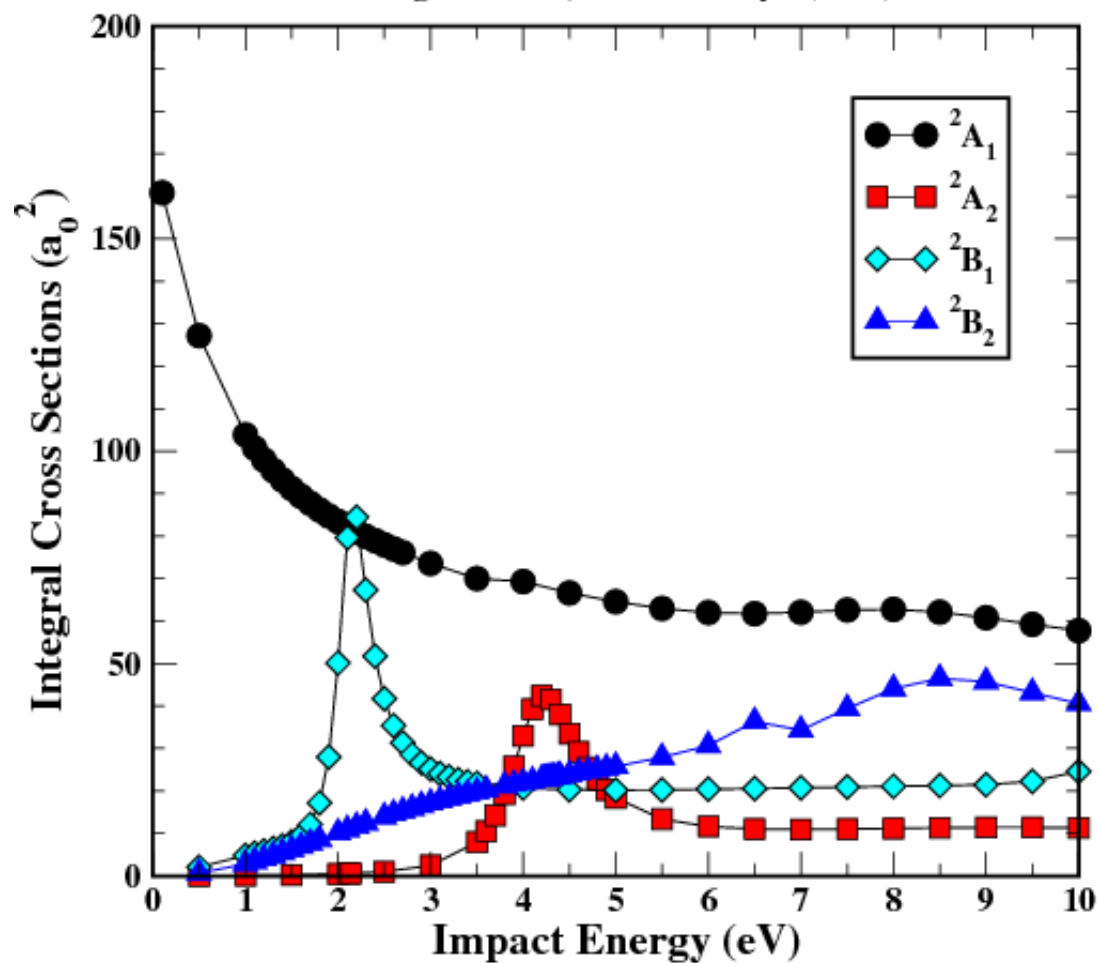
Electronic transition $X\ ^1\Sigma_g^+ \to a'\ ^1\Sigma_u^-$ of N_2 by electron impact
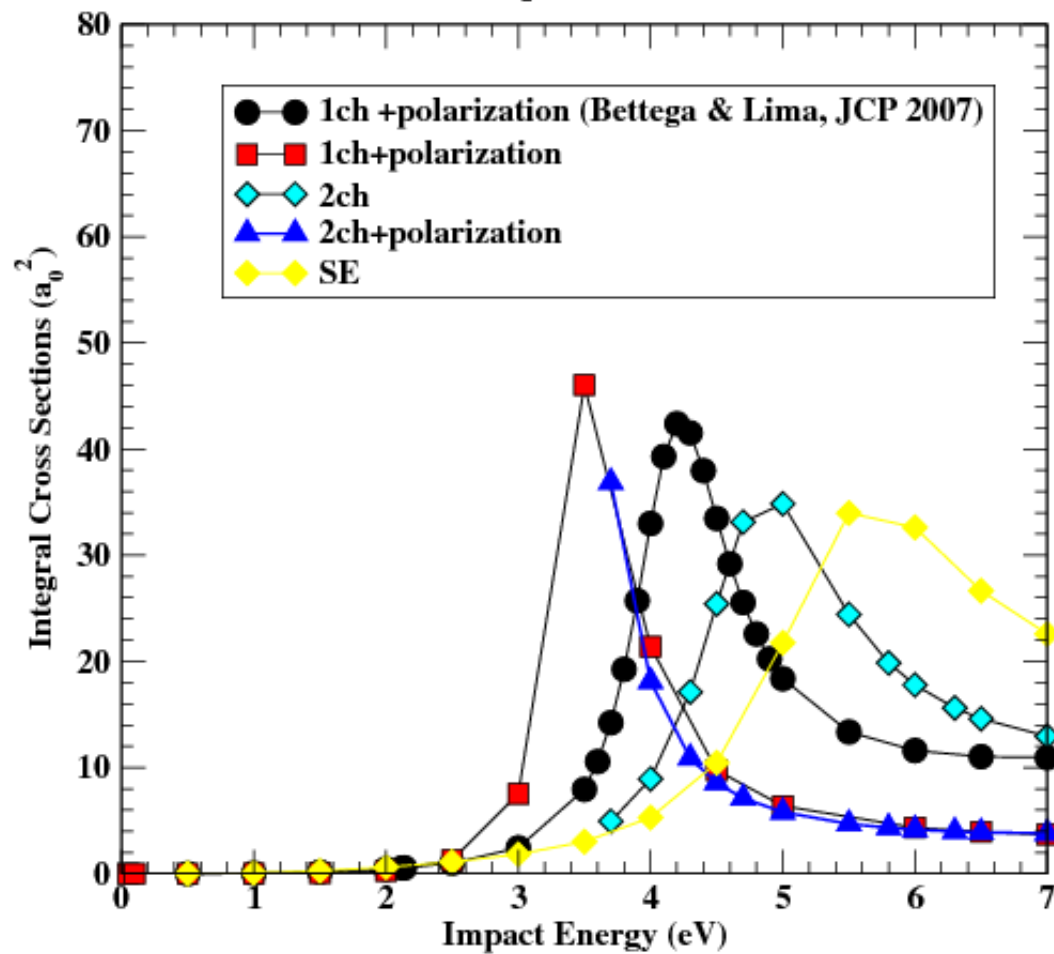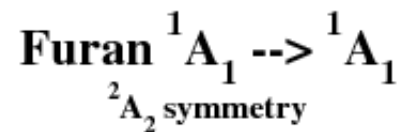
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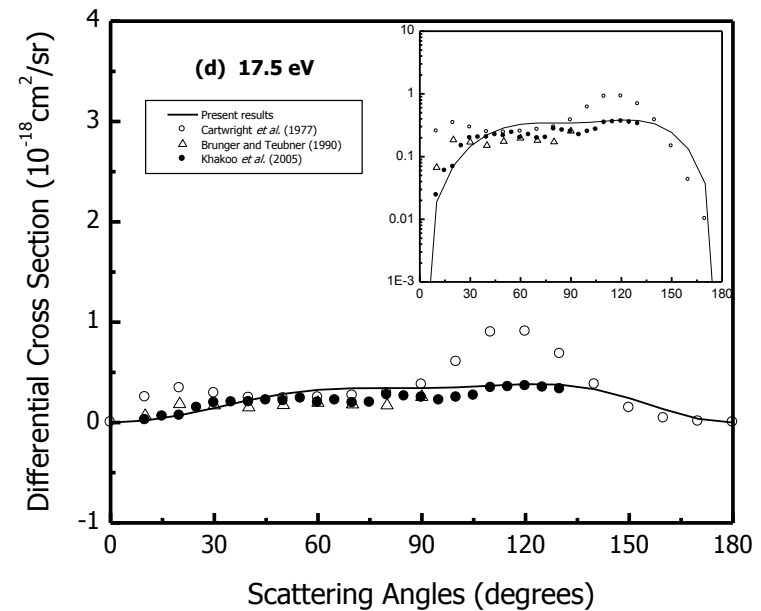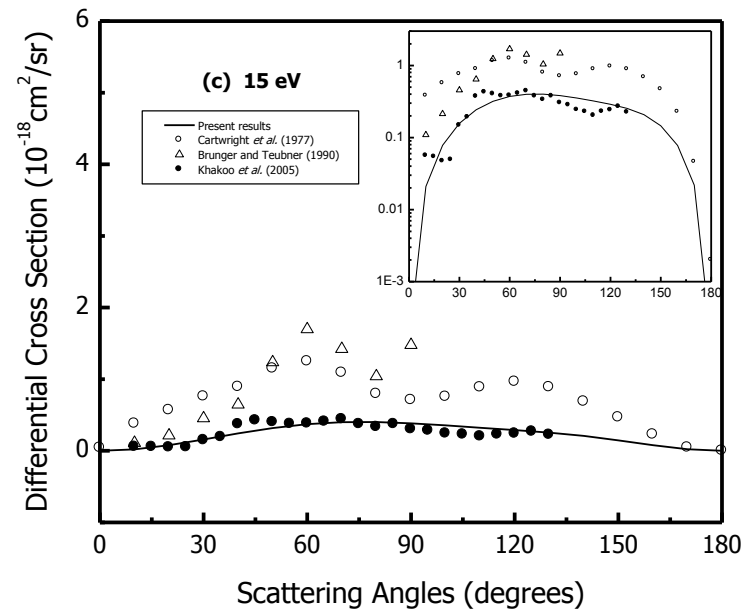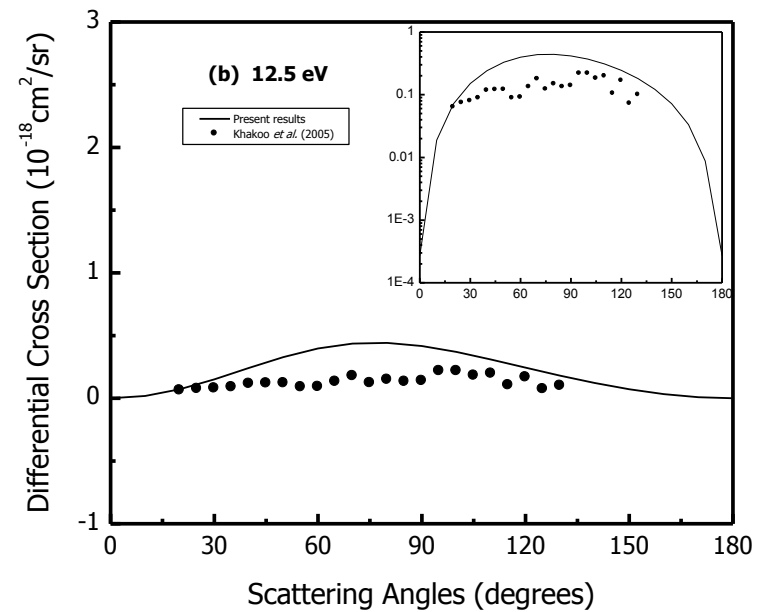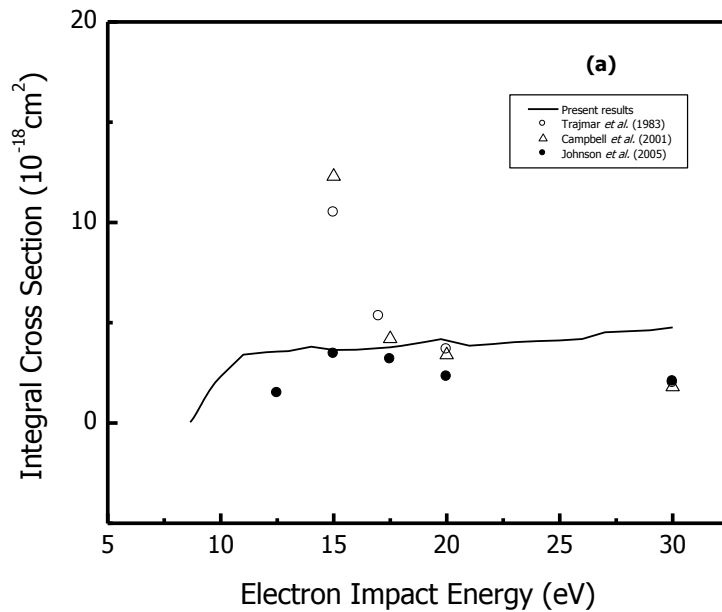
Are polarization effects important in electronic excitation?

Electron-Furan Scattering

Bettega & Lima, J. Chem. Phys. (2007)

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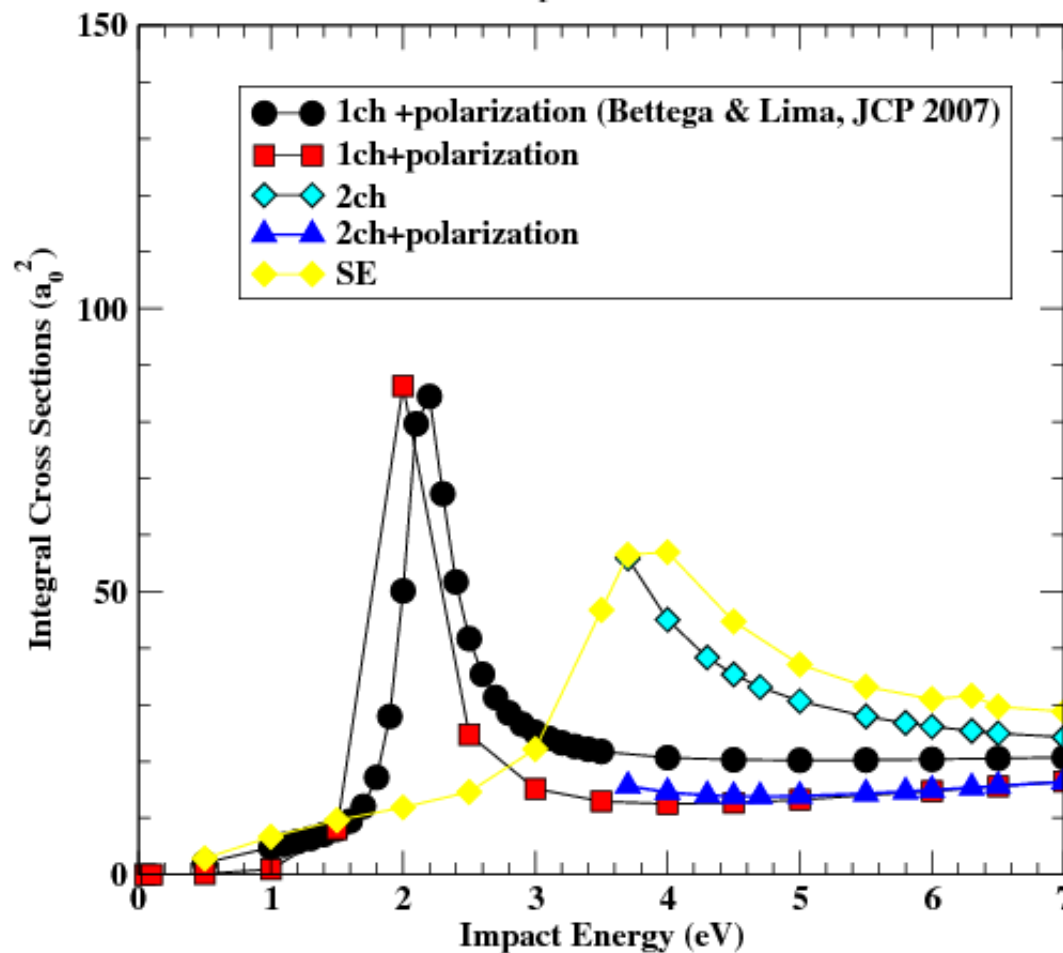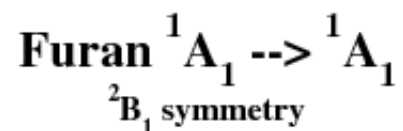Instituto de Física Gleb Wataghin
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Resonance's positions change with polarization effects

Furan $^1A_1$ --> $^1A_1$
$^2A_2$ symmetry

Legend:
- 1ch +polarization (Bettega & Lima, JCP 2007)
- 1ch+polarization
- 2ch
- 2ch+polarization
- SE

Threshold of $^3B_2$ state ↑

R. F. da Costa, M. H. F. Bettega, and M. A. P. Lima, *Phys. Rev. A* **77**, 012717 (2008).

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Resonance's positions change with polarization effects

Threshold of $^3B_2$ state

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66

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Polarization effects change excitation cross sections

Furan $^1A_1 \rightarrow {}^3B_2$
$^2A_2$ symmetry

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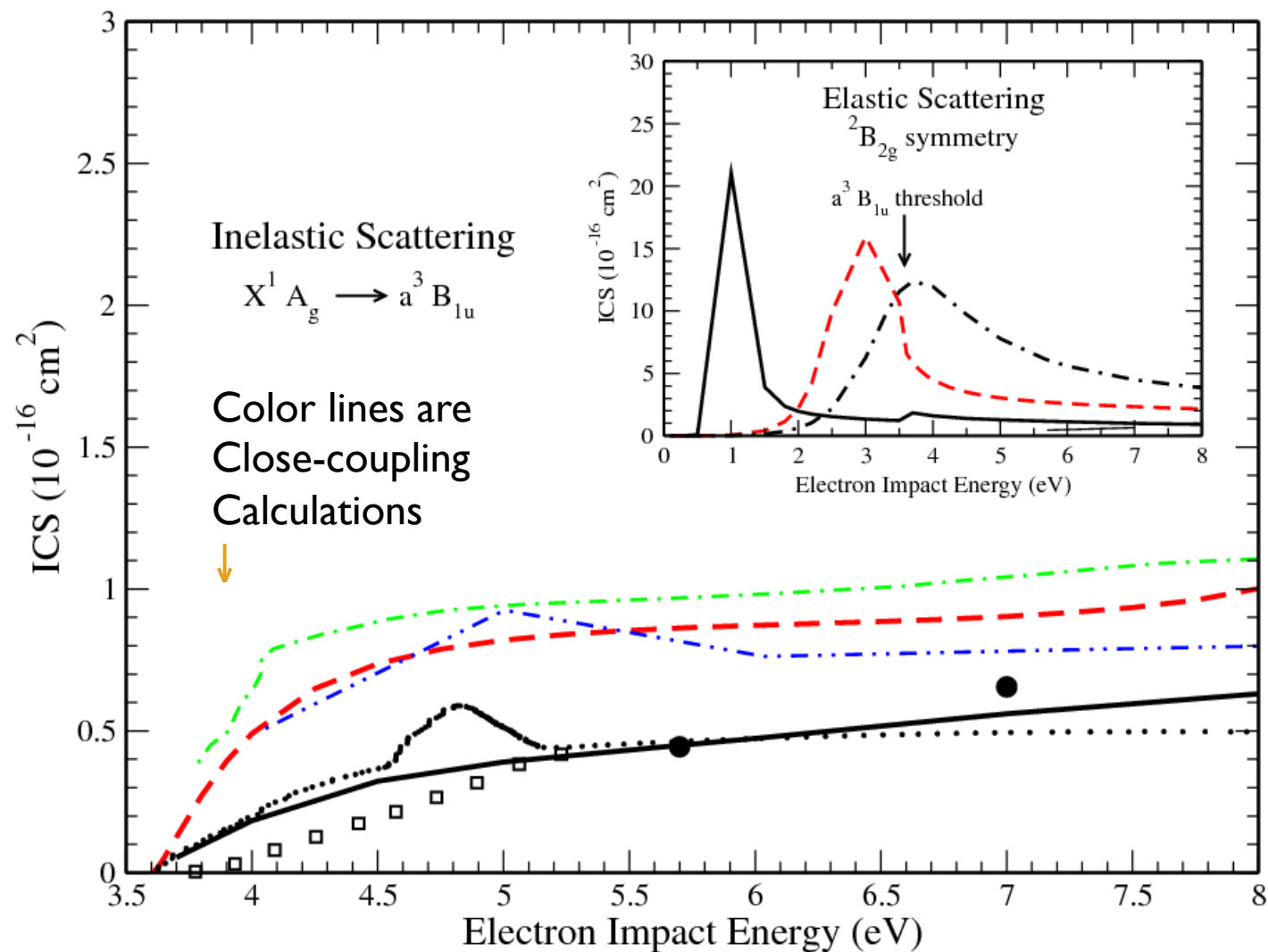
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67

MAPLima
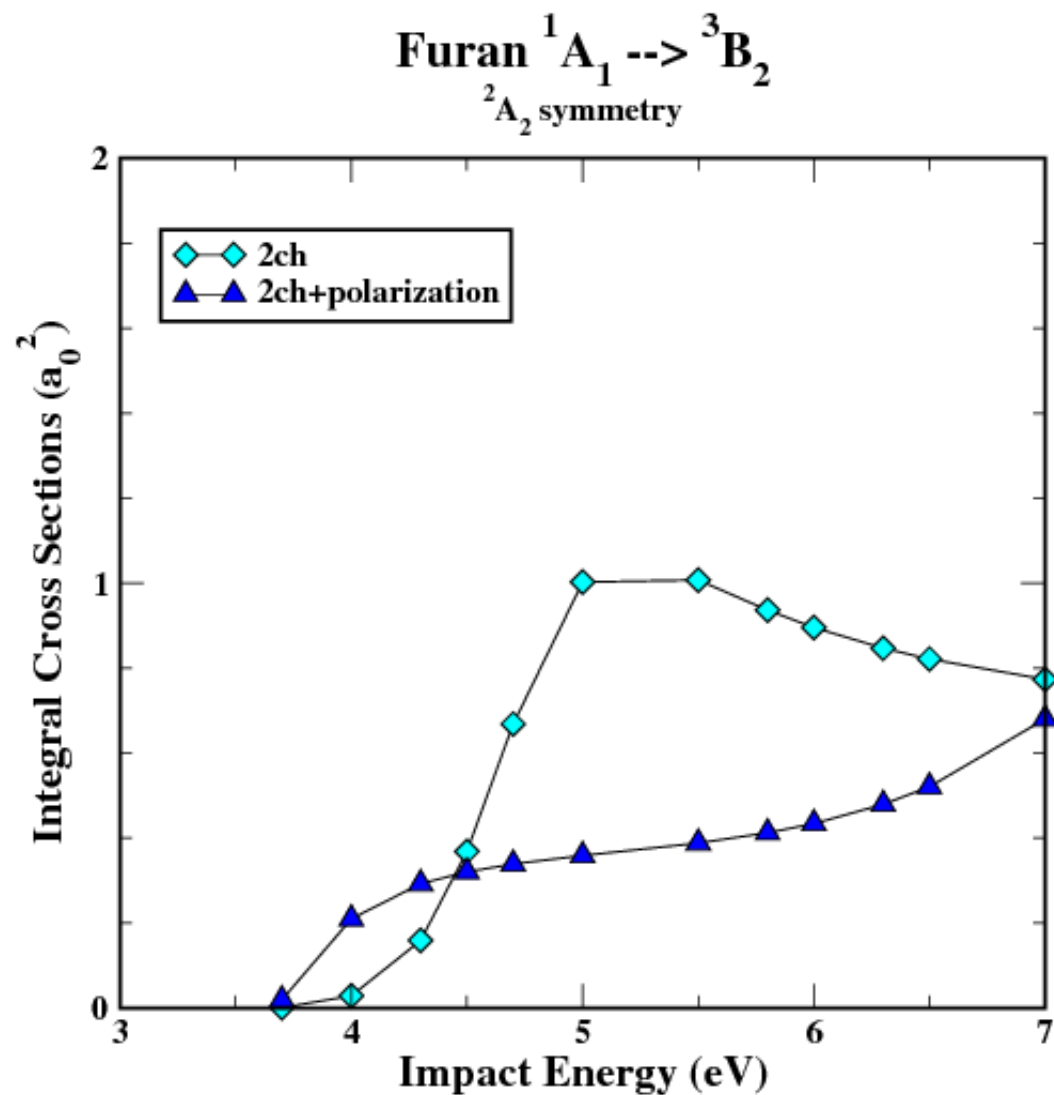
Resonance's positions change the excitation dynamics

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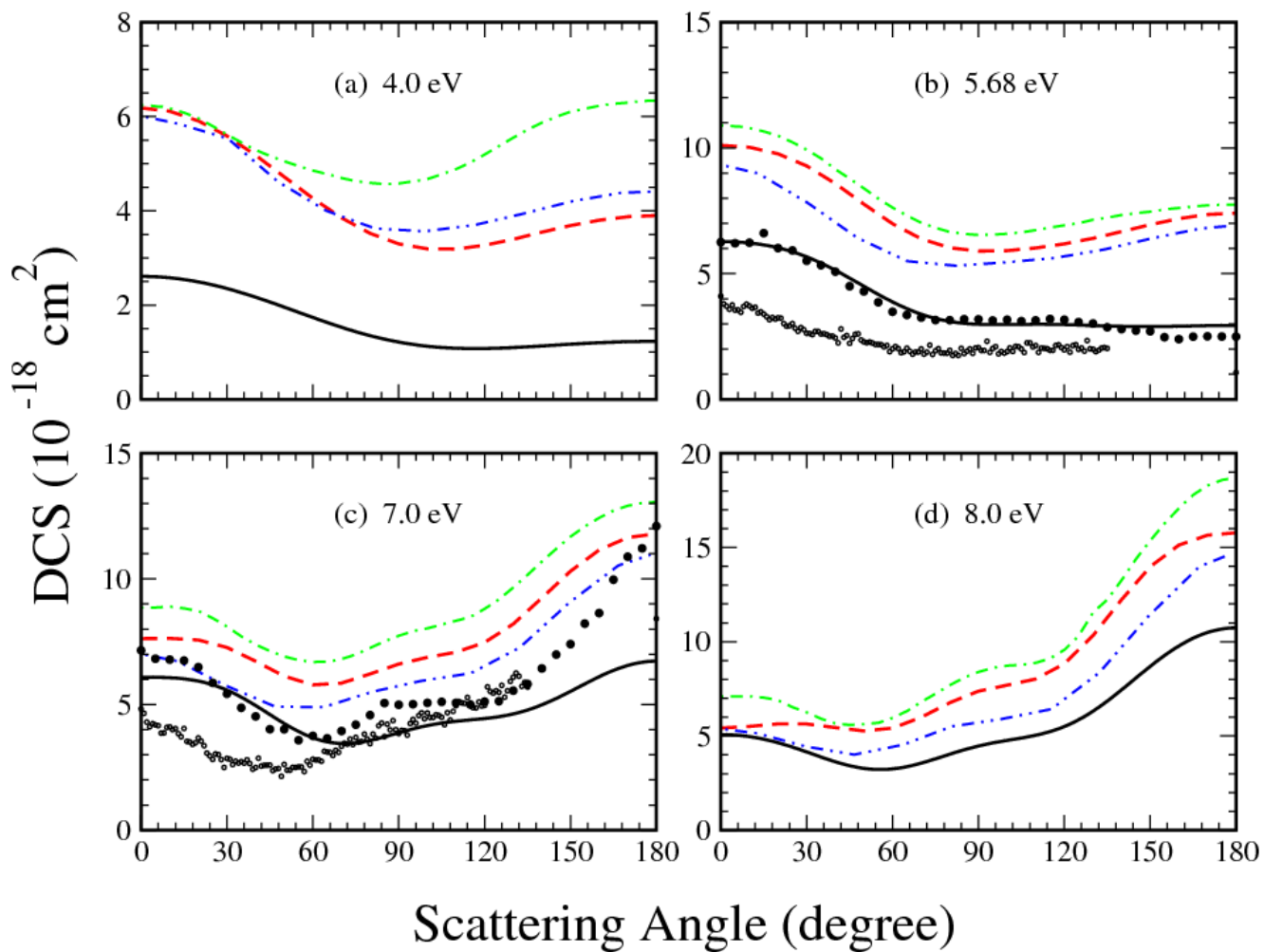
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Electronic excitation of ã $^3B_{1u}$ state of C_2H_4 by electron impact

Inelastic Scattering

$$X^1 A_g \longrightarrow a^3 B_{1u}$$

Color lines are
Close-coupling
Calculations

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70

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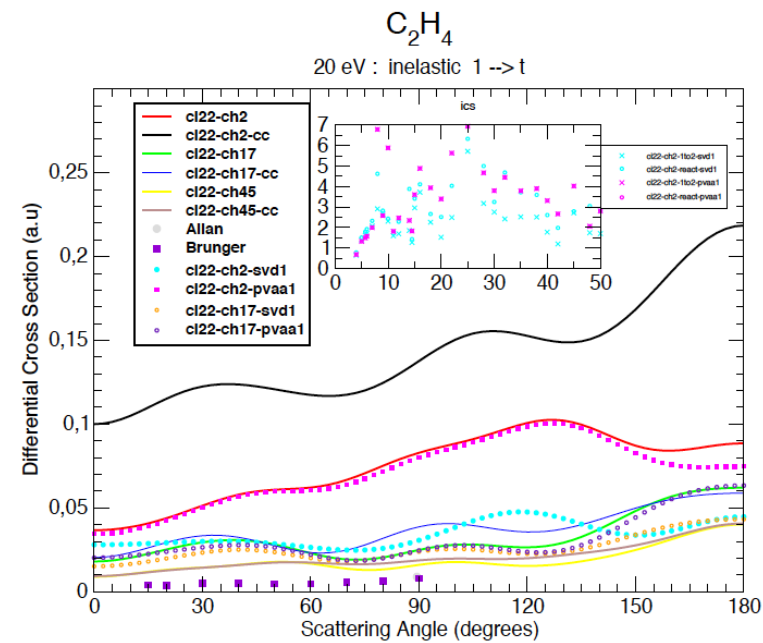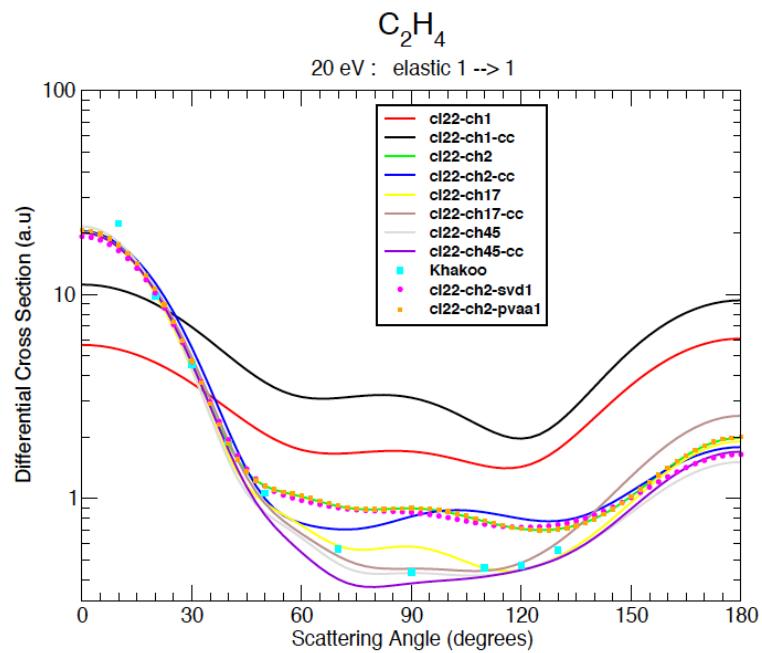## Electronic excitation of ã $^3B_{1u}$ state of C_2H_4 by electron impact

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

MAPLima
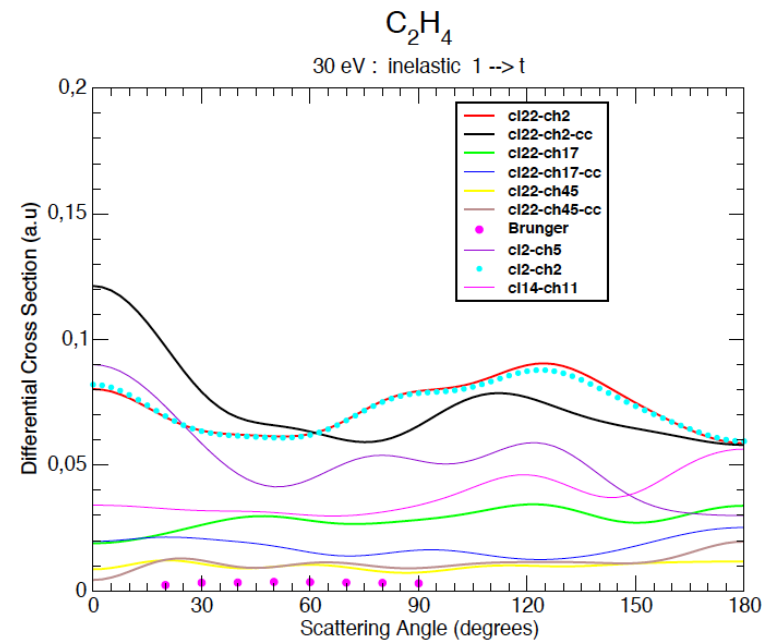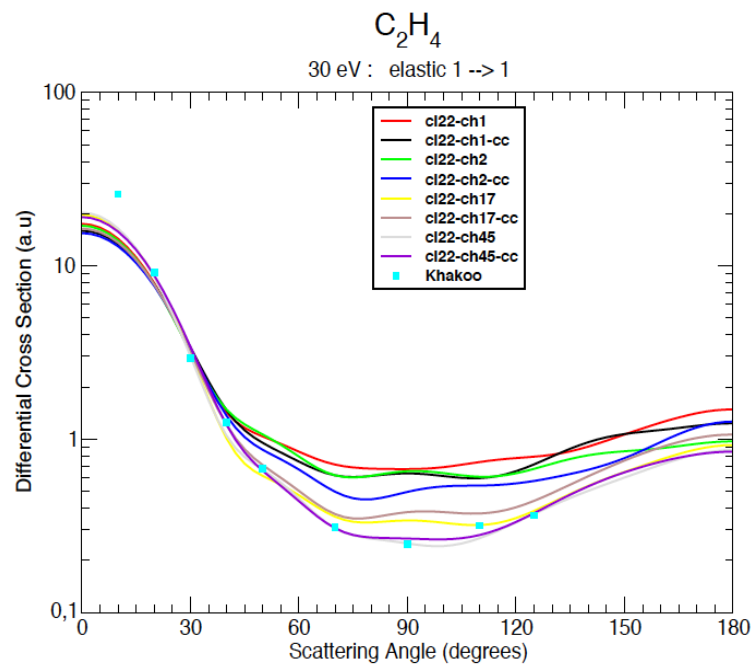
Thank you very much for your attention

A copy of this presentation is at
http://www.ifi.unicamp.br/~maplima/maplima-xiwfme2013.pdf