APS physics

Electron Scattering by biomass molecular fragments

by
Marco A. P. Lima
Unicamp

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68th GEC
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12-16 Oct. 15
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REVIEWING MOTIVATIONS

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From the 80's up to now these scientific topics and applications stimulated the community

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Electron scattering by Molecules

DISCHARGE ENVIROMENTS

This community was inspired by several basic science problems →

Natural Phenomena	Aurora Borealis
Astrophysics	Planetary Atmospheres
Biology	DNA dissociation … Plasma Science towards Future Medicine
Quantum Optics	Molecular Lasers

and got further motivated by great applications →

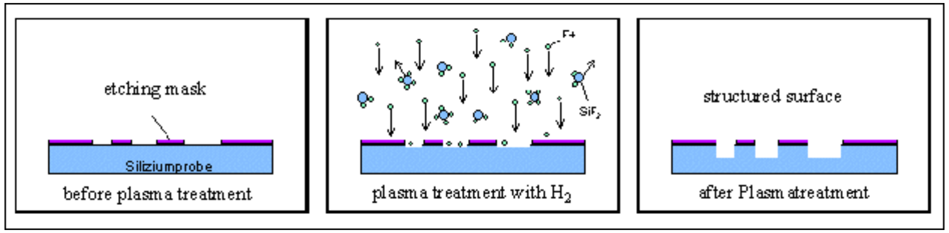
- Ozone destruction
- Control of pollution
- Sterilization $$
- Surface treatment $$$$
- Nanofabrication $$$$
- Medical treatment $$$$

Surface treatment with Plasmas

Modeling is a big challenge

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

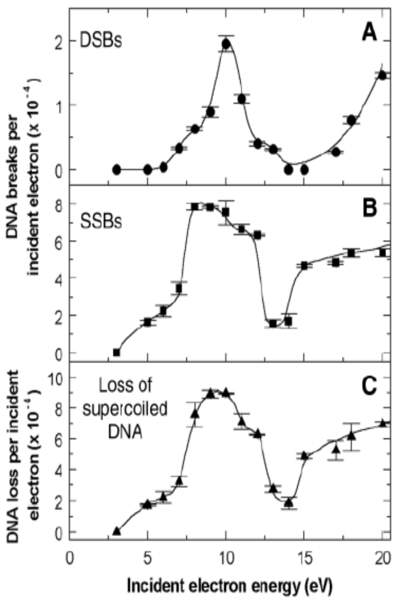
APS physics

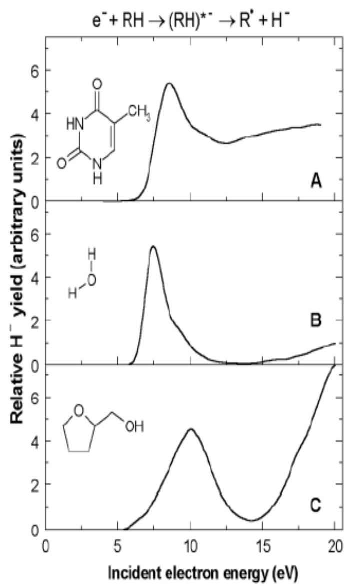
Resonance's inducing dissociation.
How precise the data (position and width) must be?

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





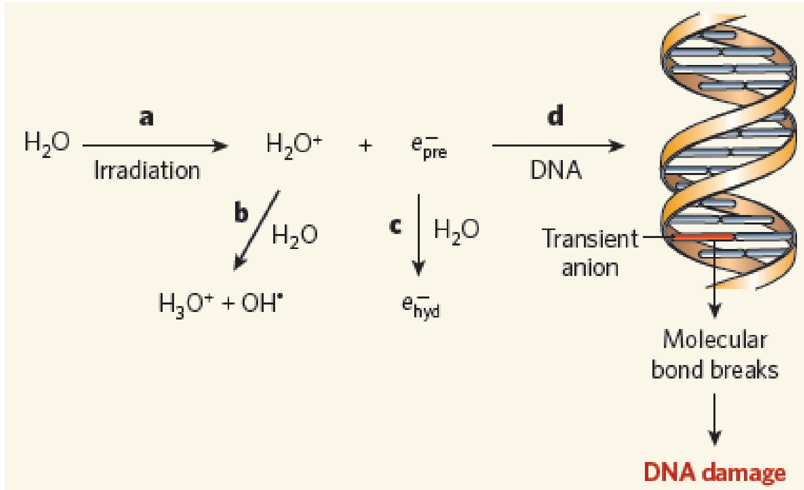
Science, **287** 1658 (2000)

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

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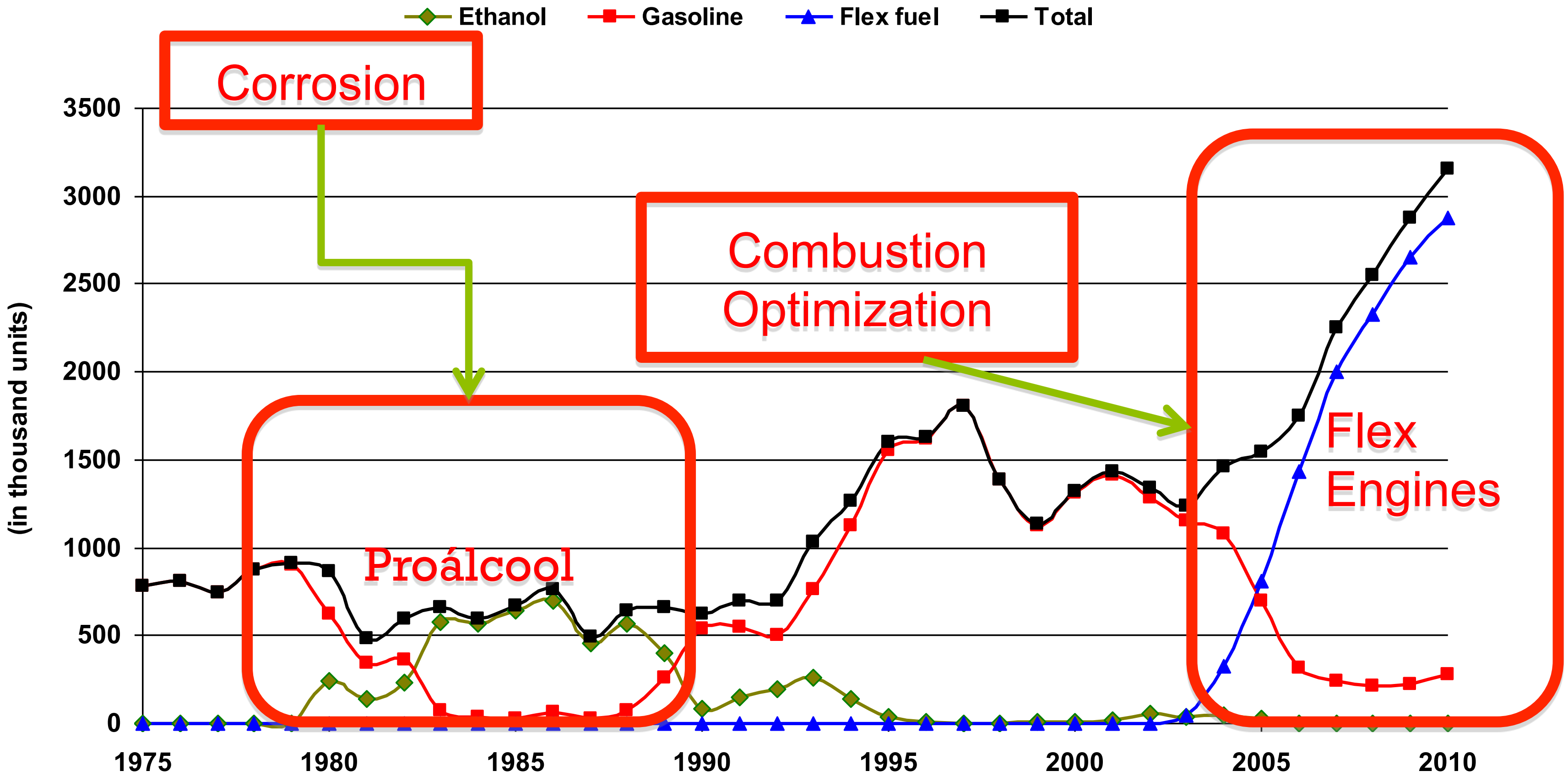
SPECIAL MOTIVATION

Special 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

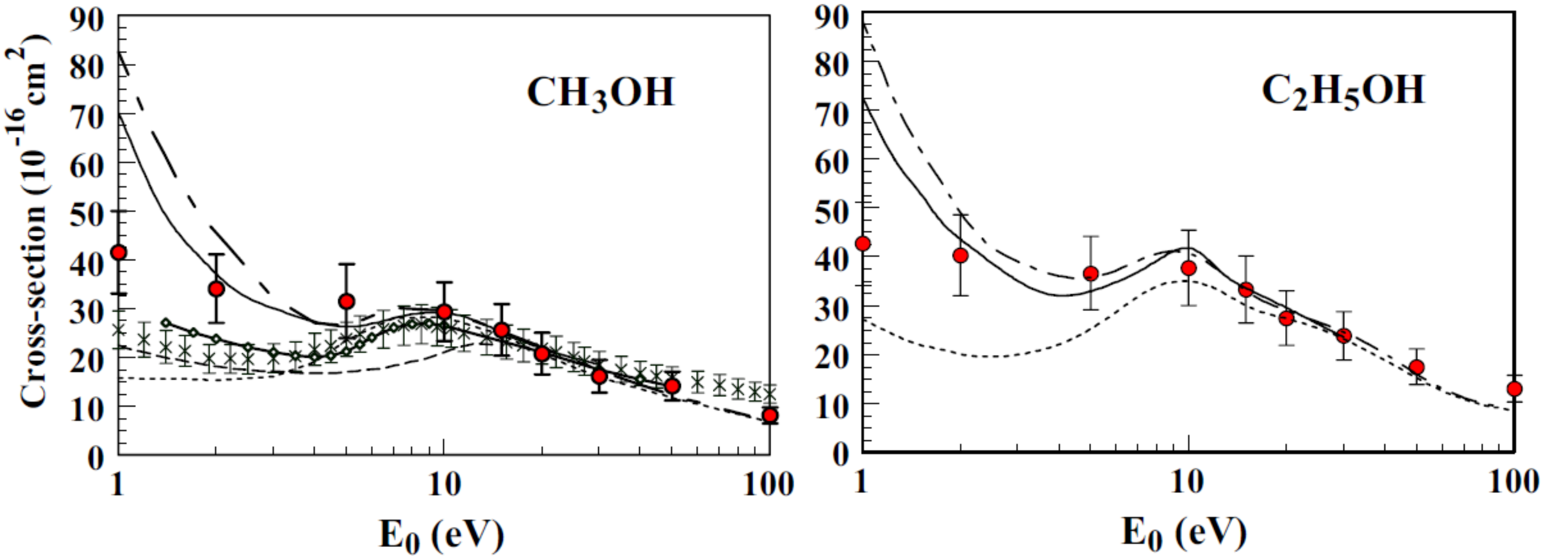
Theoretical support for an application project working on:

- 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 elastic scattering from methanol and ethanol,

M. A. Khakoo, J. Blumer, K. Keane, C. Campbell, H. Silva, M. C. A. Lopes, C. Winstead, V. Mckoy, R. F. da Costa, L. G. Ferreira, M. A. P. Lima, and M. H. F. Bettega, *Phys. Rev. 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.

Other molecules like propanol, butanol and pentanol were also studied.

NSF (Caltech/Fullerton)/CNPq (Unicamp/UFJF/UFPR/USP/UFABC) project

Special motivation II: large scale production of ethanol

A sugarcane industry of Sugar/Ethanol/Bioeletricity

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Special motivation II: large scale production of ethanol

Biomass: a source of energy and carbon

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Special motivation II: large scale production of ethanol

Biomass: a source of energy and carbon

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Special motivation II: large scale production of ethanol

First generation ethanol: crushing the cane for the juice

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Special motivation II: large scale production of ethanol

Bagasse piles at the mill.

2nd generation ethanol?
Other high value bioproducts?

Can we use plasmas on Biomass?

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The motivation of a theoretician

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

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Theoretical background

Scattering theory

See review: "Recent advances in the application of the Schwinger multichannel method with pseudopotentials to electron-molecule collisions", R. F. da Costa, M. T. do N. Varella, M.H.F. Bettega, and M.A.P. Lima, *Eur. Phys. J. D* **69**, 1 (2015).

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

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

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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

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

Schwinger Variational Principle

The Schwinger Variational method serves to get a scattering amplitude free of first order errors for a scattering process that respect the equations

$$A^{(\pm)}|\Psi^{(\pm)}_{\mathbf{k}}\rangle = V|S_{\mathbf{k}}\rangle \text{ and } \begin{cases} f_{\mathbf{k_f},\mathbf{k_i}} = \langle S_{\mathbf{k_f}}|V|\Psi^{(+)}_{\mathbf{k_i}}\rangle \\ f_{\mathbf{k_f},\mathbf{k_i}} = \langle \Psi^{(-)}_{\mathbf{k_f}}|V|S_{\mathbf{k_i}}\rangle \\ f_{\mathbf{k_f},\mathbf{k_i}} = \langle \Psi^{(-)}_{\mathbf{k_f}}|A^{(+)}|\Psi^{(+)}_{\mathbf{k_i}}\rangle \end{cases} \text{ and } A^{(\pm)} = V - VG_0^{(\pm)}V$$

The bilinear form of the variational principle for the scattering amplitude is $[f_{\mathbf{k_f},\mathbf{k_i}}] = \langle S_{\mathbf{k_f}}|V|\Psi^{(+)}_{\mathbf{k_i}}\rangle + \langle \Psi^{(-)}_{\mathbf{k_f}}|V|S_{\mathbf{k_i}}\rangle - \langle \Psi^{(-)}_{\mathbf{k_f}}|A^{(+)}|\Psi^{(+)}_{\mathbf{k_i}}\rangle$ where arbitrary and independent variations with respect to

$$\begin{cases} \langle \delta\Psi^{(-)}_{\mathbf{k_f}}|\left(V|S_{\mathbf{k_i}}\rangle - A^{(+)}|\Psi^{(+)}_{\mathbf{k_i}}\rangle\right) = 0 \\ \left(\langle S_{\mathbf{k_f}}|V - \langle \Psi^{(-)}_{\mathbf{k_f}}|A^{(+)}\right)|\delta\Psi^{(+)}_{\mathbf{k_i}}\rangle = 0 \end{cases}$$

lead to

$$\begin{cases} V|S_{\mathbf{k_i}}\rangle - A^{(+)}|\Psi^{(+)}_{\mathbf{k_i}}\rangle = 0 \Rightarrow A^{(+)}|\Psi^{(+)}_{\mathbf{k_i}}\rangle = V|S_{\mathbf{k_i}}\rangle \\ \langle S_{\mathbf{k_f}}|V - \langle \Psi^{(-)}_{\mathbf{k_f}}|A^{(+)} = 0 \Rightarrow A^{(-)}|\Psi^{(-)}_{\mathbf{k_f}}\rangle = V|S_{\mathbf{k_f}}\rangle \text{ with } {A^{(+)}}^\dagger = A^{(-)} \end{cases}$$

$A^{(\pm)}|\Psi^{(\pm)}_{\mathbf{k}}\rangle = V|S_{\mathbf{k}}\rangle$ *is equivalent to* $H|\Psi^{(\pm)}_{\mathbf{k}}\rangle = E|\Psi^{(\pm)}_{\mathbf{k}}\rangle$ *with proper boundary conditions.*

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

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

It is the same for all transitions

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

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

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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 , $j \geq 2$ 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

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Coupling level

Inelastic scattering with and without polarization

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

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

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

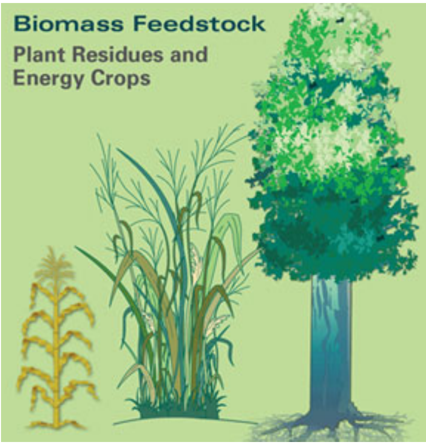
❷ Again the configuration space is made of

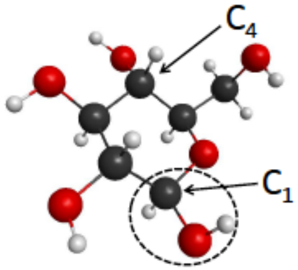
$$|\chi_\mu\rangle = \begin{cases} a_{N+1}\,|\Phi_o\rangle \otimes |\varphi_i\rangle \\ a_{N+1}\,|\Phi_j\rangle \otimes |\varphi_k\rangle,\ j \geq 2 \end{cases}$$

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

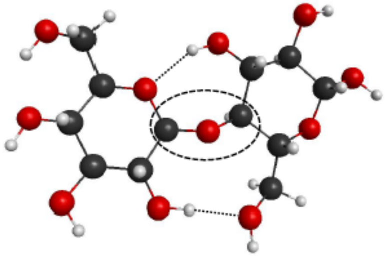
Polarization effects are included with j greater than the number of open channels

Biomass is Made Up with Fermentable Sugars

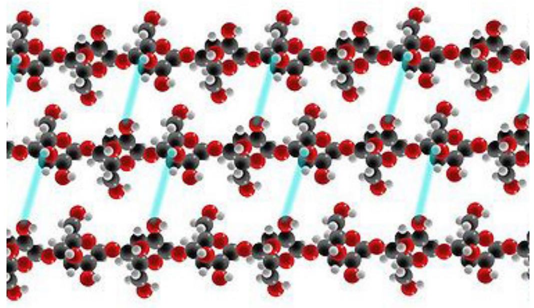


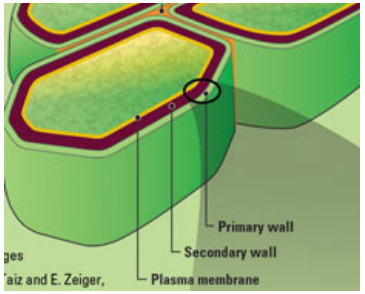


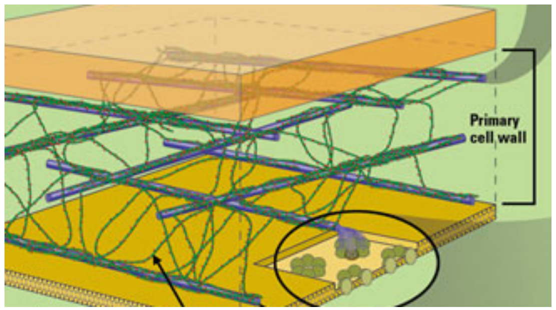
β-D-glucose

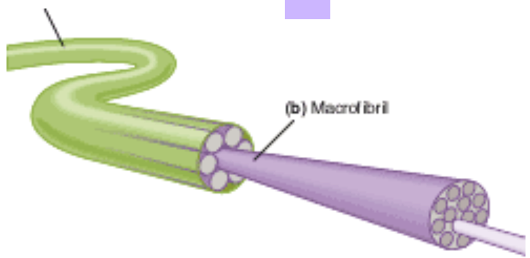


cellobiose









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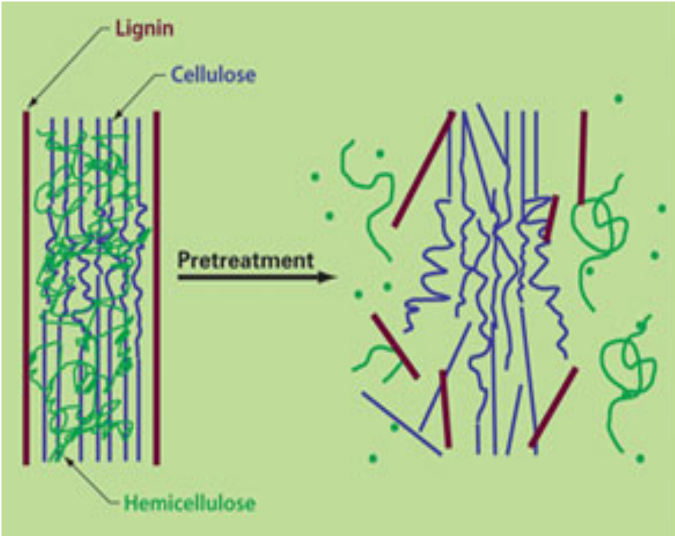
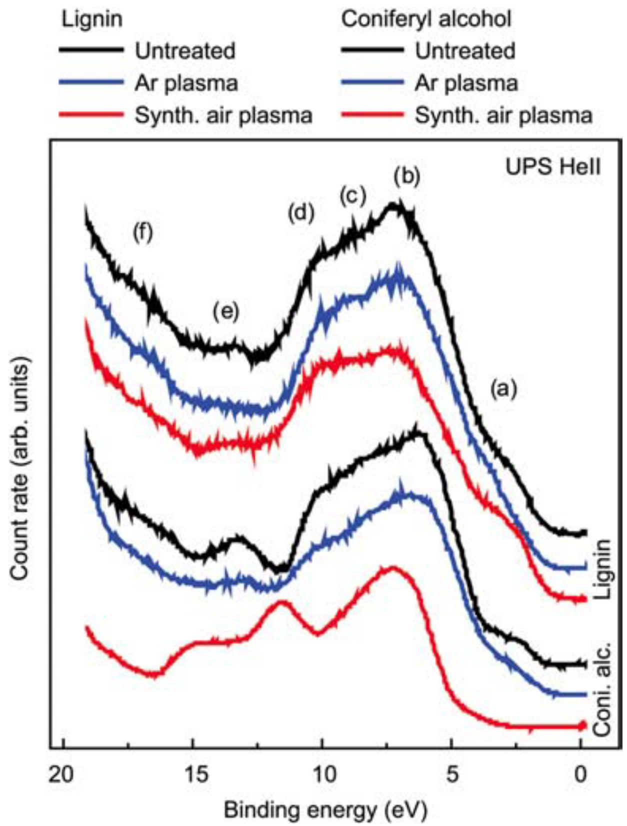
Lignocellulose is Resistant to Hydrolysis

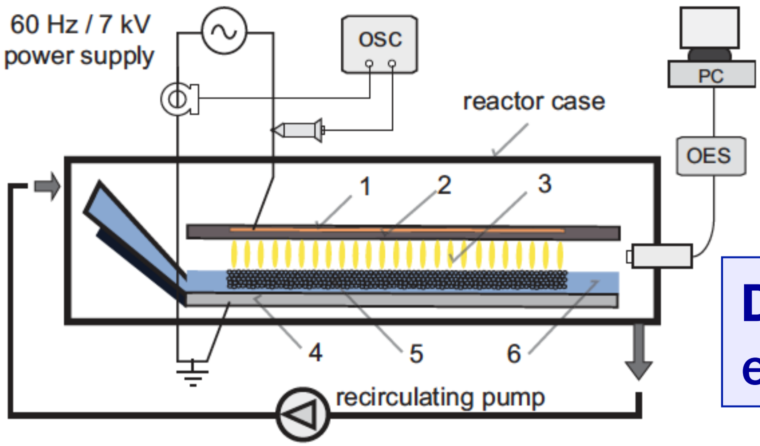


Pretreatment: bio- and physical-chemical processes to expose the cellulose fibers



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}

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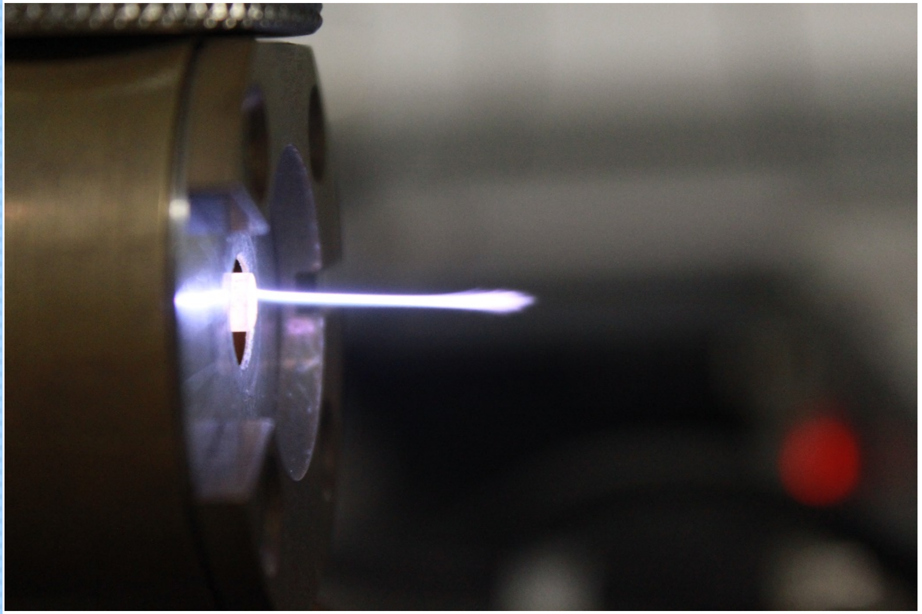
Experimental Initiative

supported by BIOEN FAPESP

- Microwave Plasmas in argon at atmospheric pressure
- Exploration of their potential for applications, in particular, to the treatment of biomass (sugar cane bagasse)



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

Diffuse Reflectance Fourier Transform Infrared Spectrometry (DRIFT)

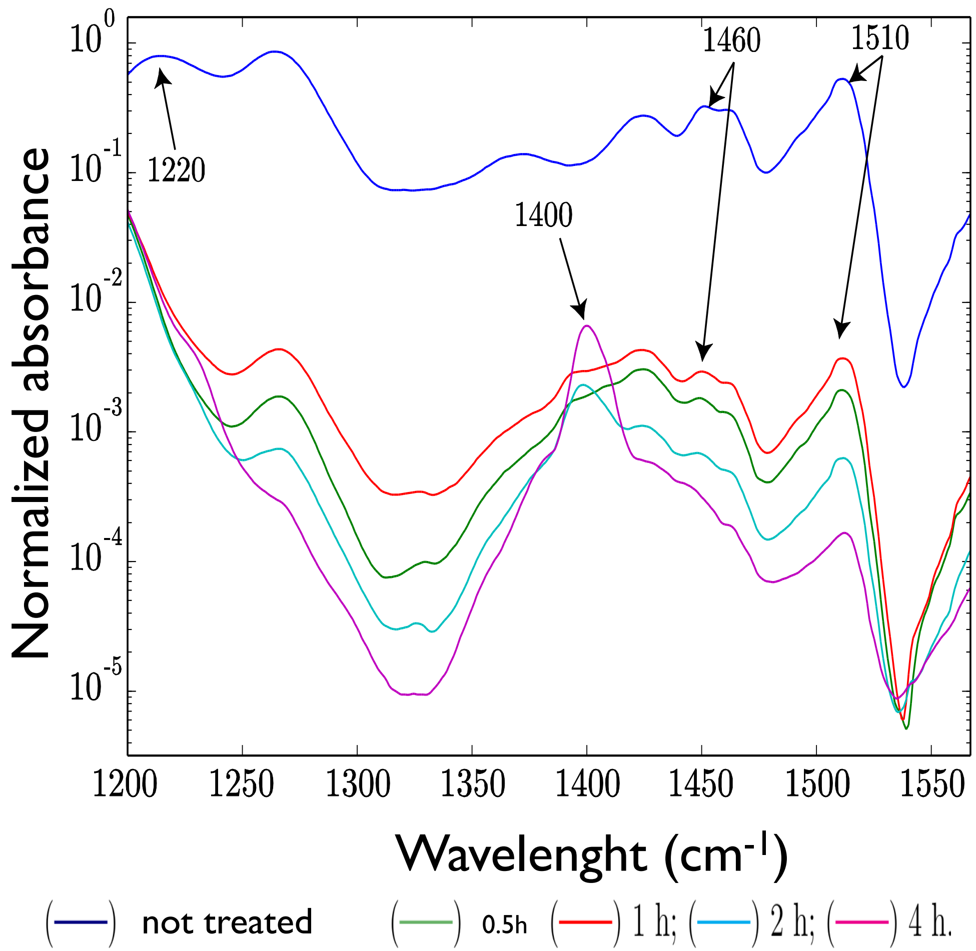
wavelenght:

1220 cm^{-1}

CC plus CO plus CO stretching in Guaiacyl group

1460 cm^{-1}

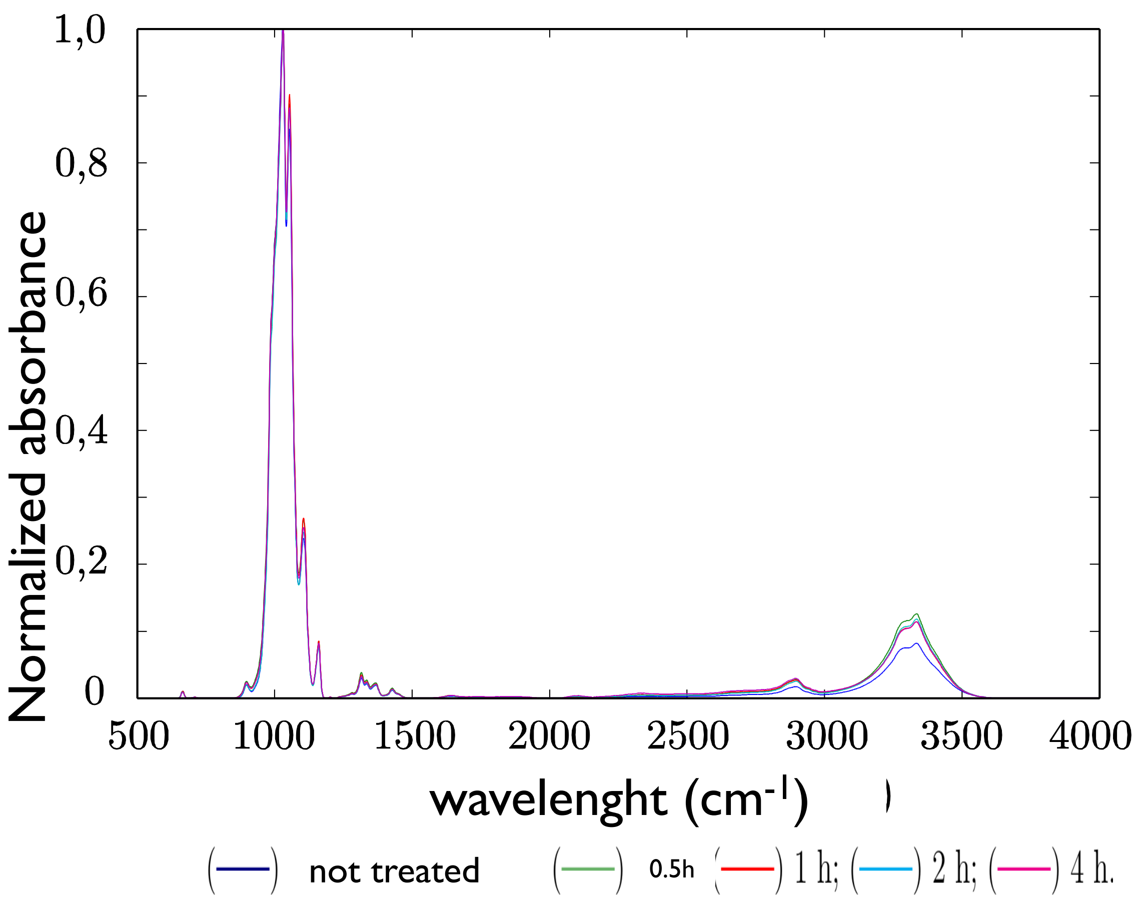
CH deformations (bend) methoxyl; asymmetric stretching in $–CH_3$ and $–CH_2$



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

Diffuse Reflectance Fourier Transform Infrared Spectrometry (DRIFT)

No modification was observed in the spectra after plasma treatment on cellulose



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

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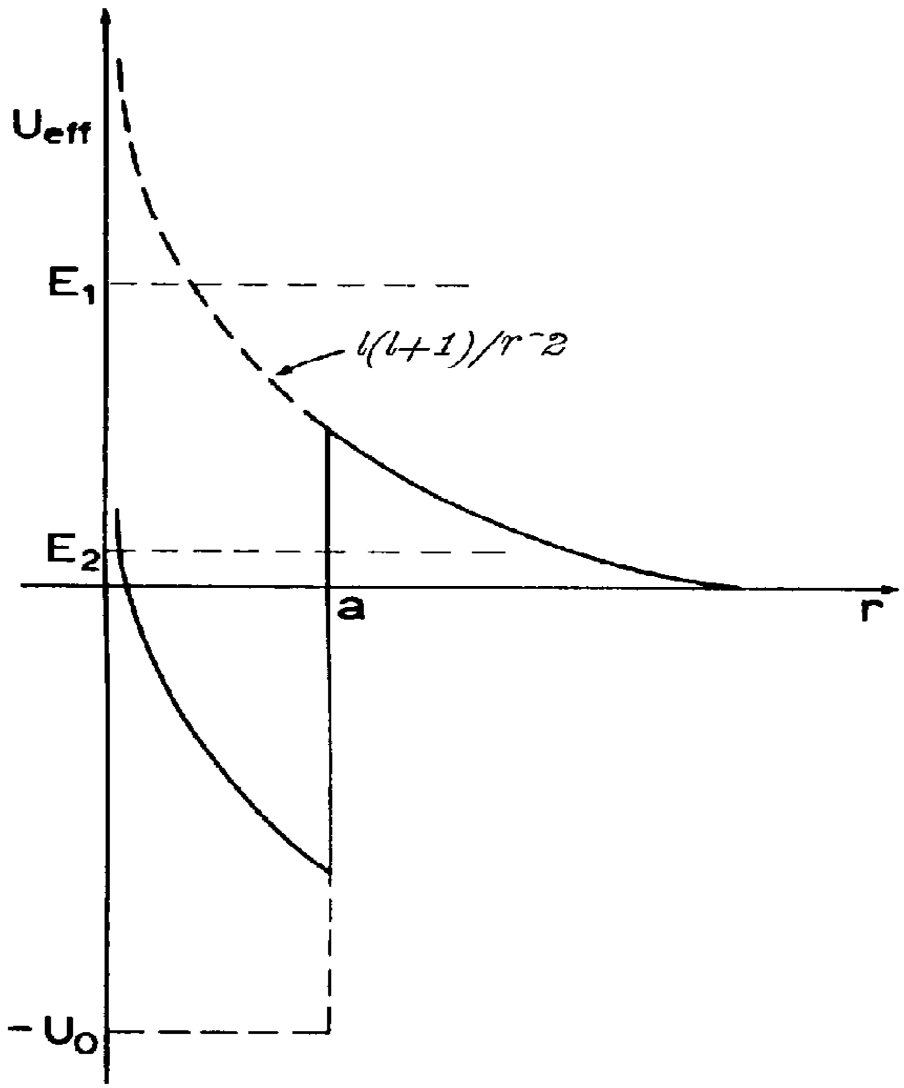
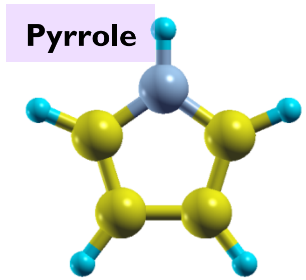
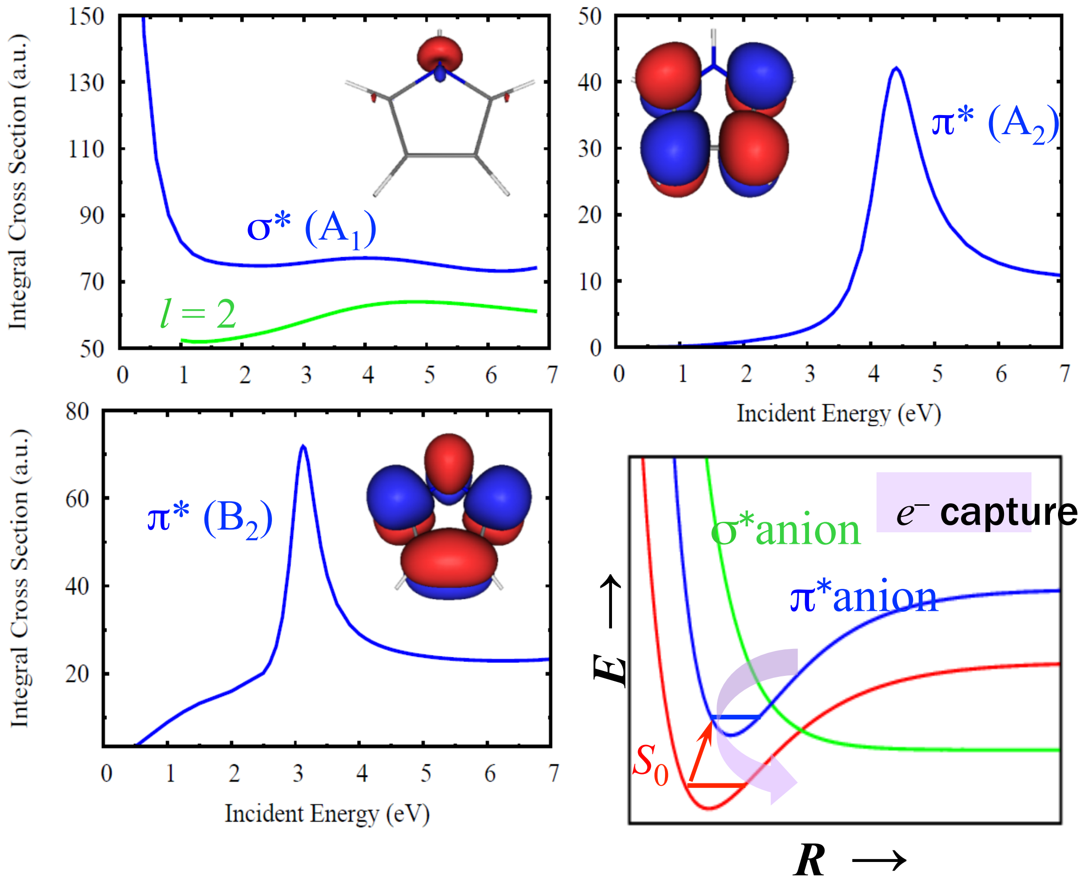
Shape resonances are related to angular momentum traps



Low energy elastic electron scattering from pirrole

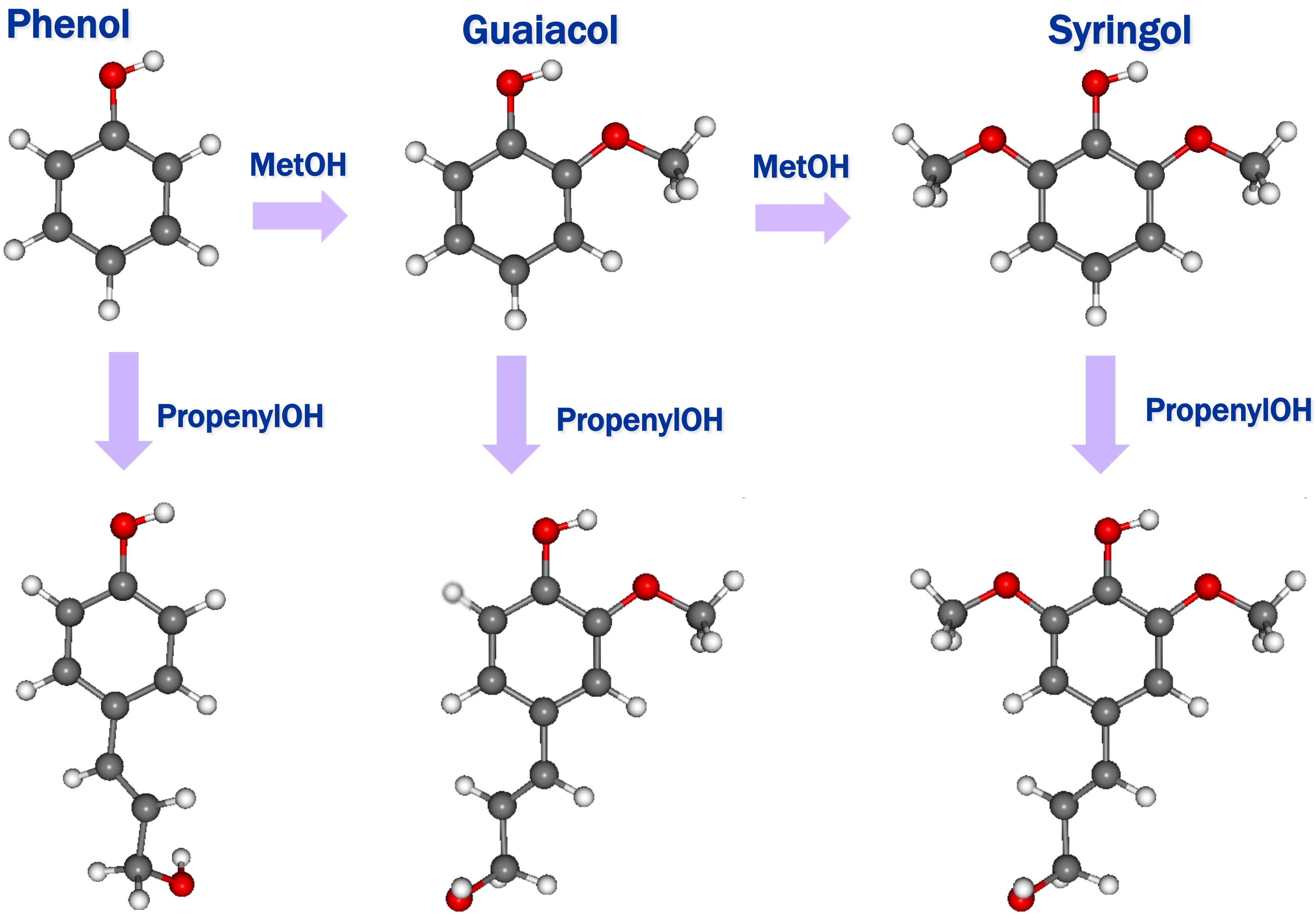
- There are π^* (ring) and σ^* (N–H) shape resonances in pyrrole. Nice prototype!





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

Lignin Subunits



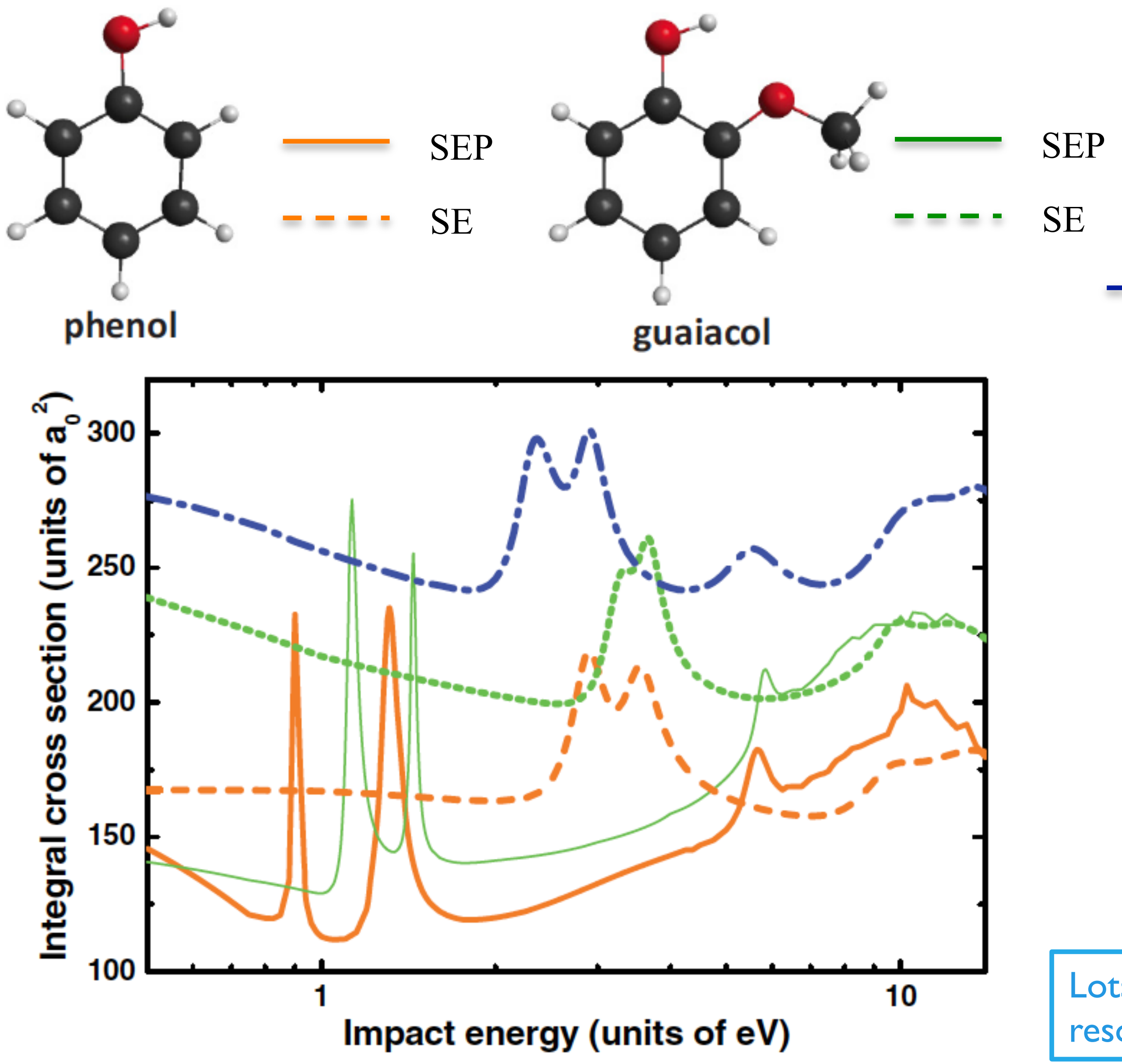
p-coumaryl alcohol   coniferyl alcohol   sinapyl alcohol

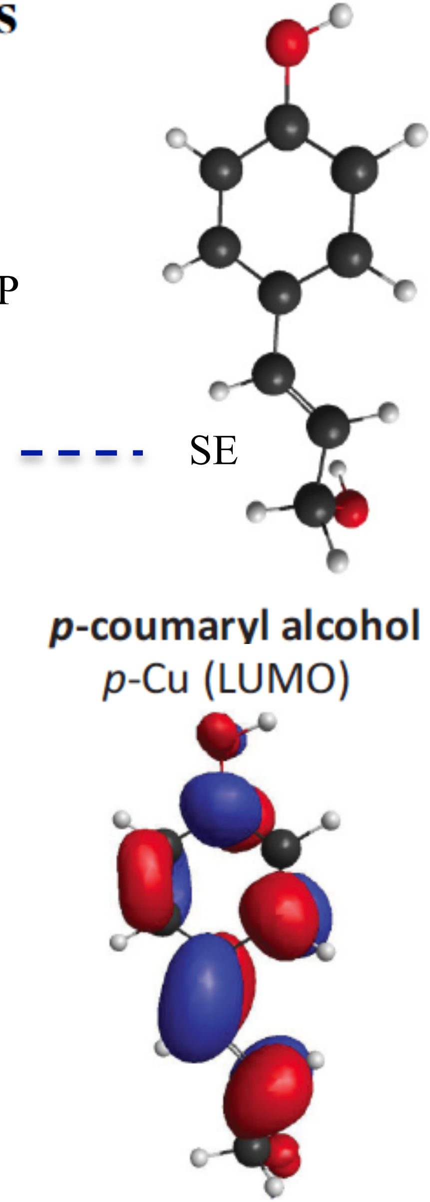
RAPID COMMUNICATIONS

Shape resonance spectra of lignin subunits

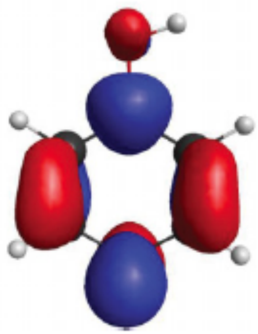
PHYSICAL REVIEW A **86**, 020701(R) (2012)

By E. M. de Oliveira, S. d'A. Sanchez, M. H. F. Bettega, A. P. P. Natalense, M. A. P. Lima, and M. T. do N. Varella.

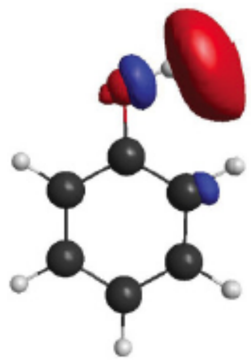




Lots of low-energy resonances!

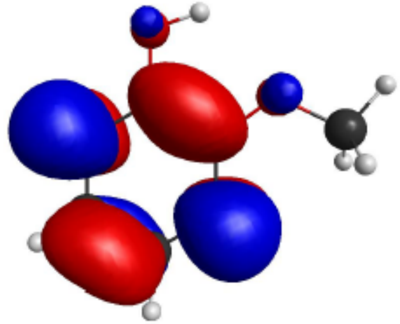


π* (LUMO+1)

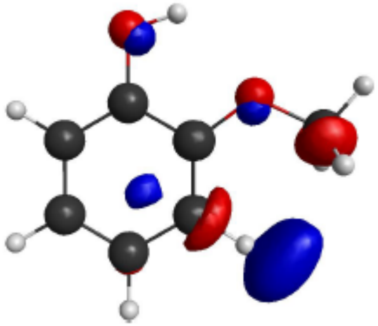


σ* (LUMO+2)

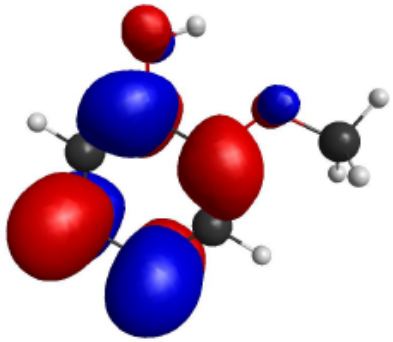
Phenol: Calculations, ET spectra and DEA data indicate H elimination from π*/σ* coupling.



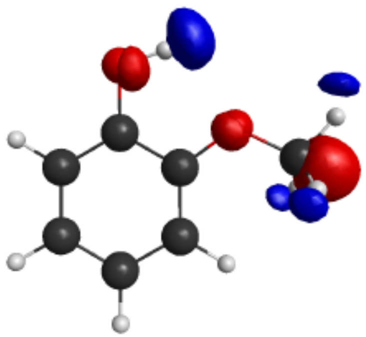
π* (LUMO)



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).

By E. M. de Oliveira, R. F. da Costa, S. d'A. Sanchez, M. H. F. Bettega, A. P. P. Natalense, M. A. P. Lima, and M. T. do N. Varella,

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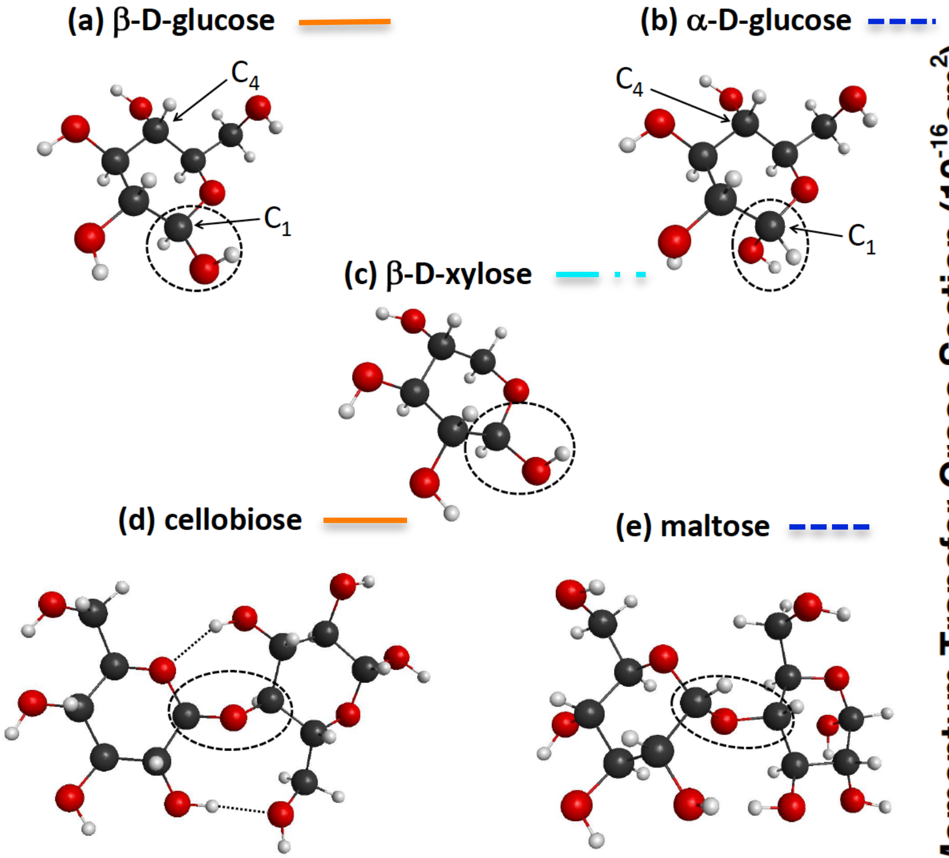

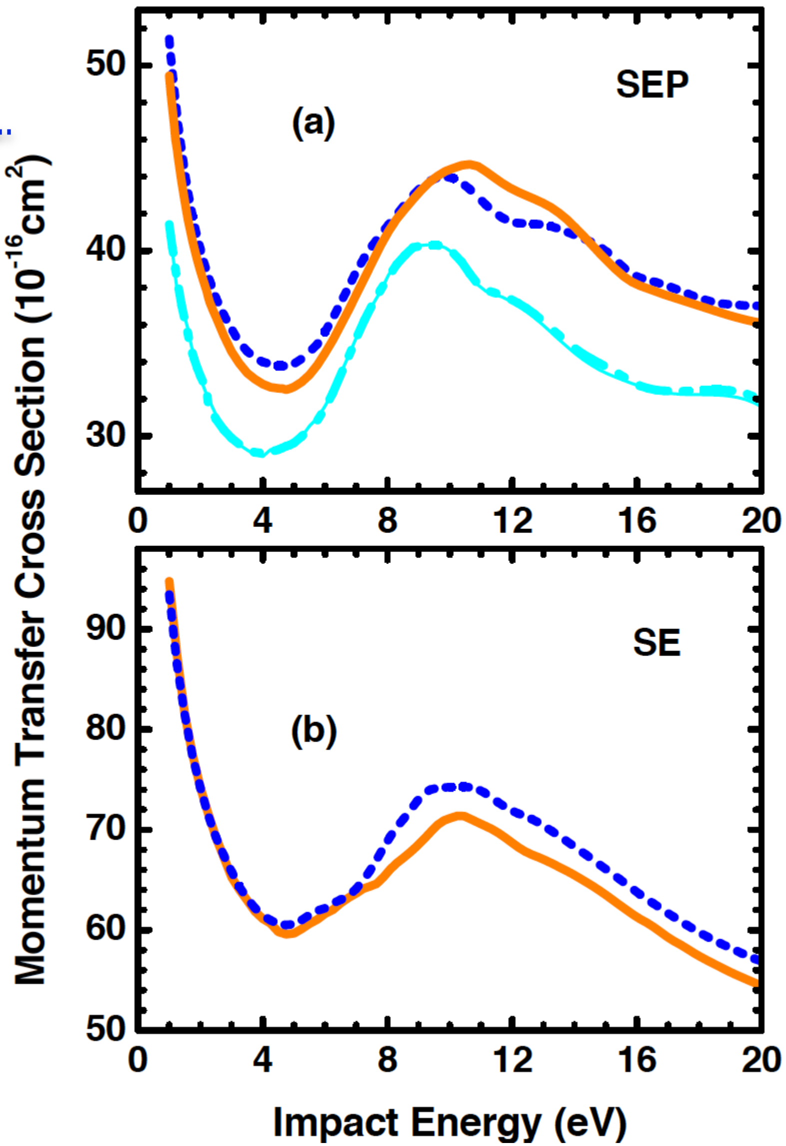

No low-energy resonances! Is this sufficient to explain why the discharge attacks the lignin and not so much the cellulose and hemicellulose?

Micro-solvation in elastic scattering

Simple first step towards more realistic situations

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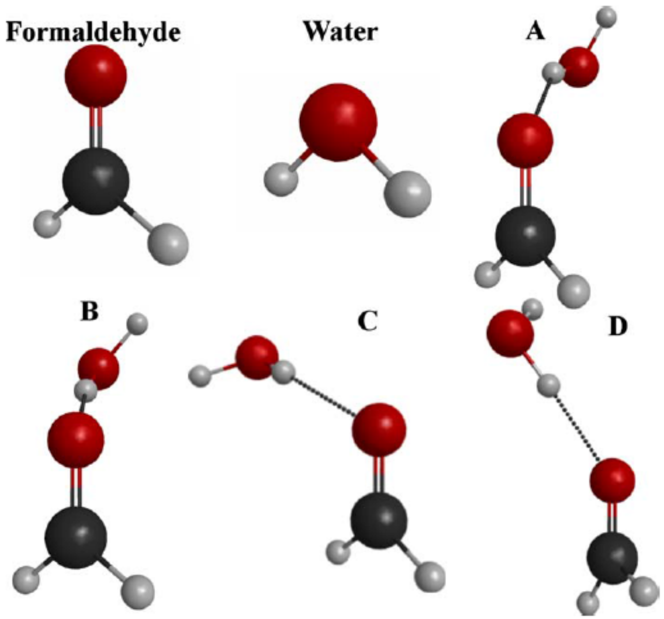
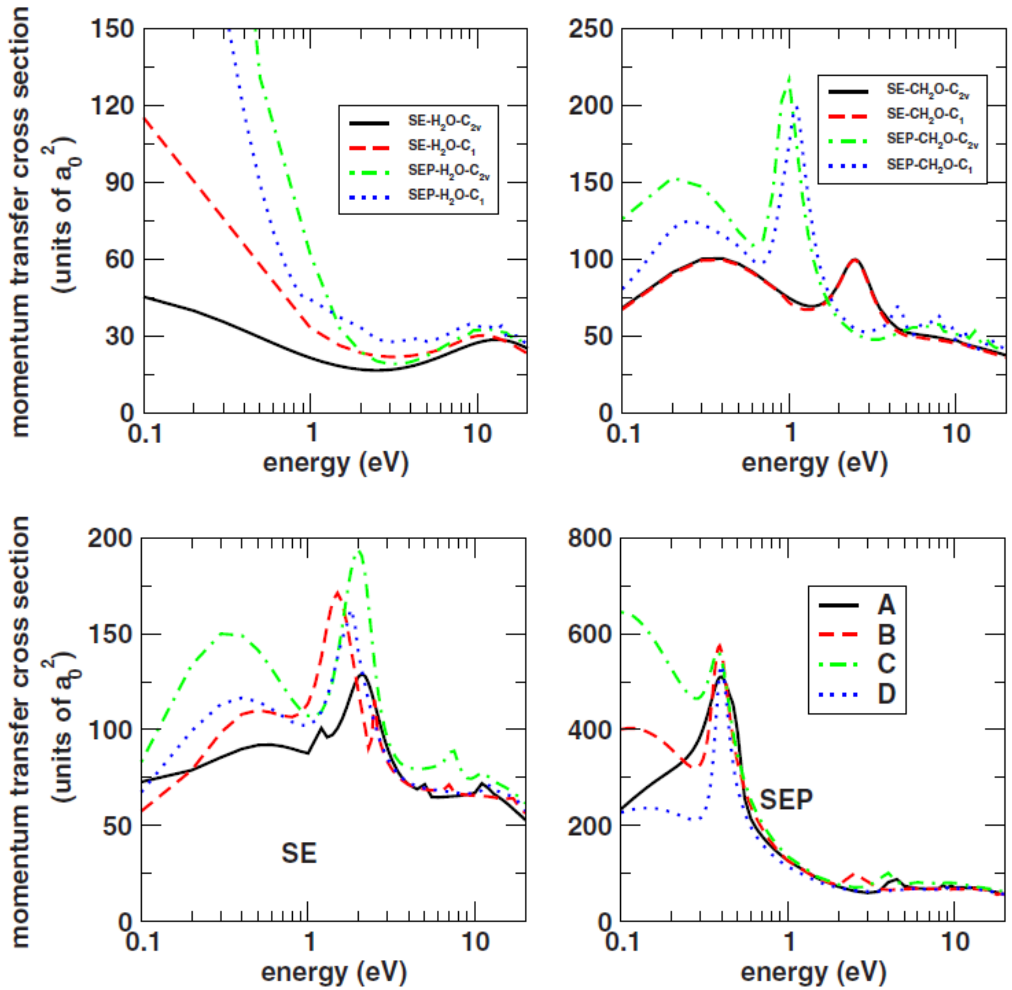
Electron Collisions with the CH_2O-H_2O complex

PHYSICAL REVIEW A 80, 062710 (2009)

By T. C. Freitas, M. A. P. Lima, S. Canuto, and M. H. F. Bettega.



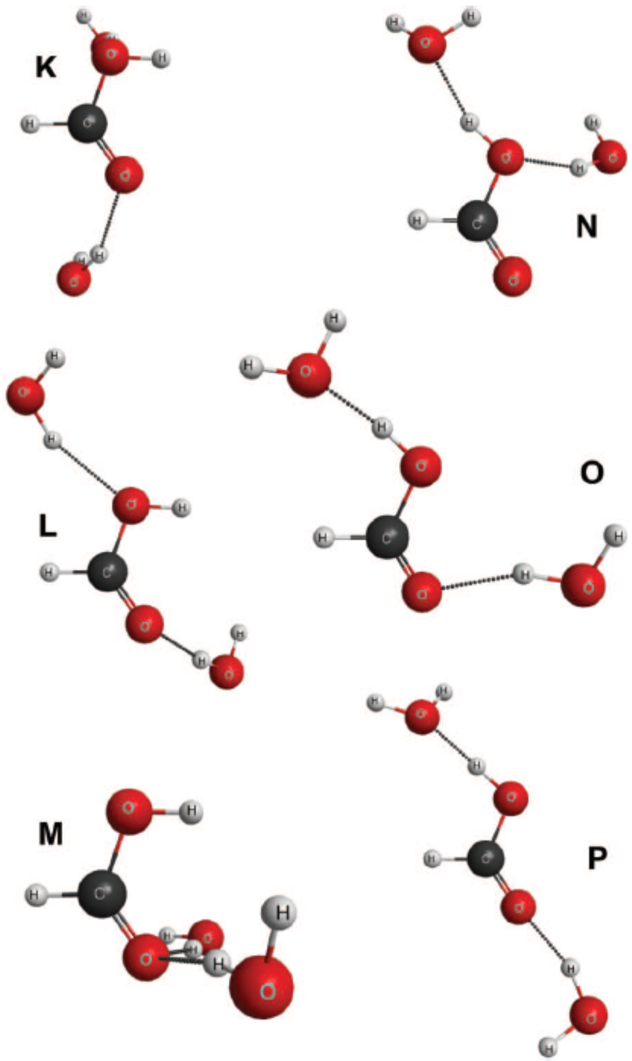


MAPLima

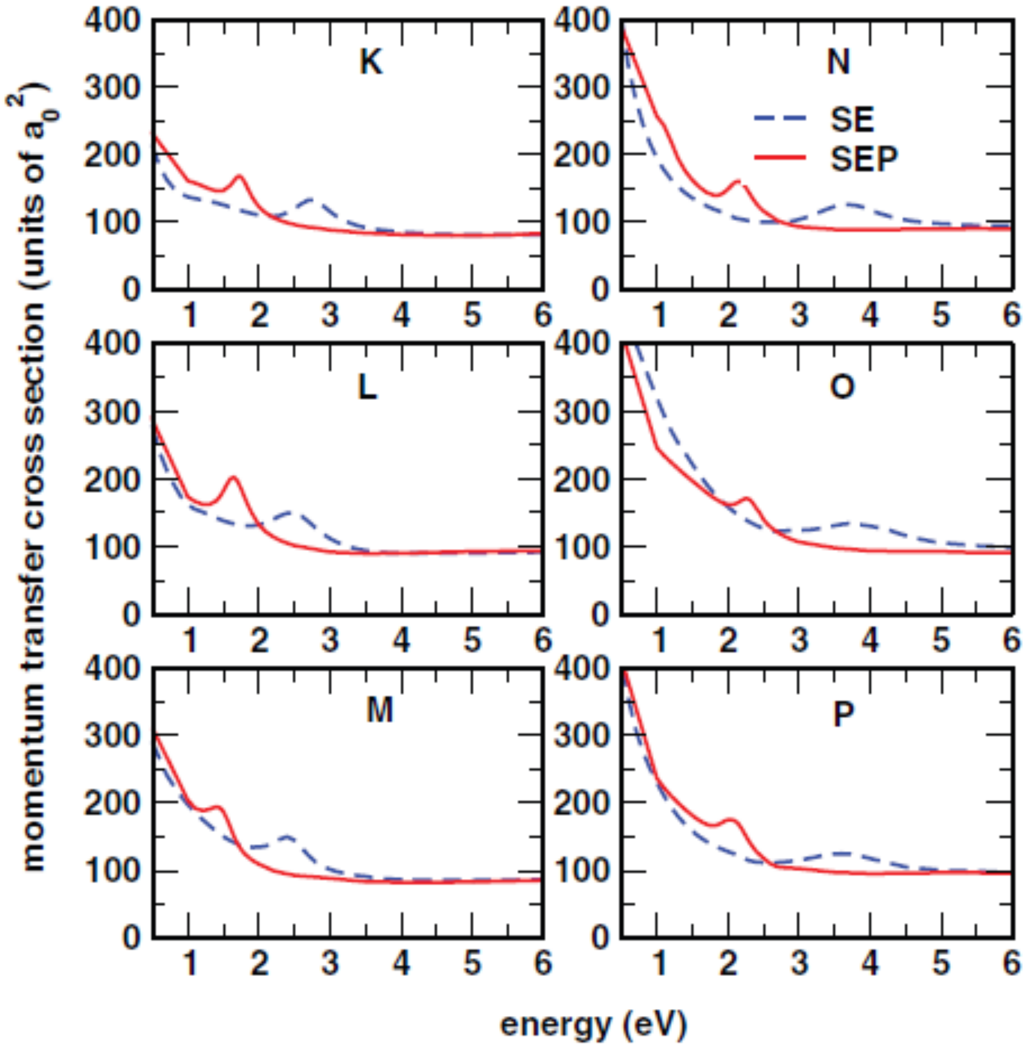
By T. C. Freitas, K. Coutinho, M. T. do N. Varella,
M. A. P. Lima, S. Canuto, M. H. F. Bettega

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)

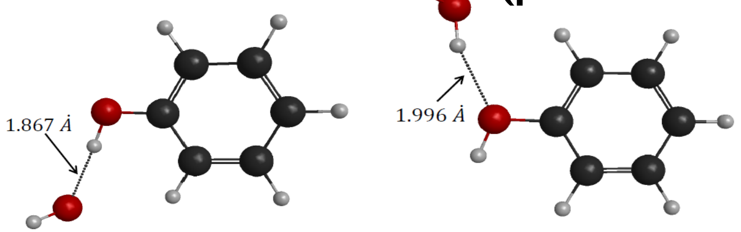


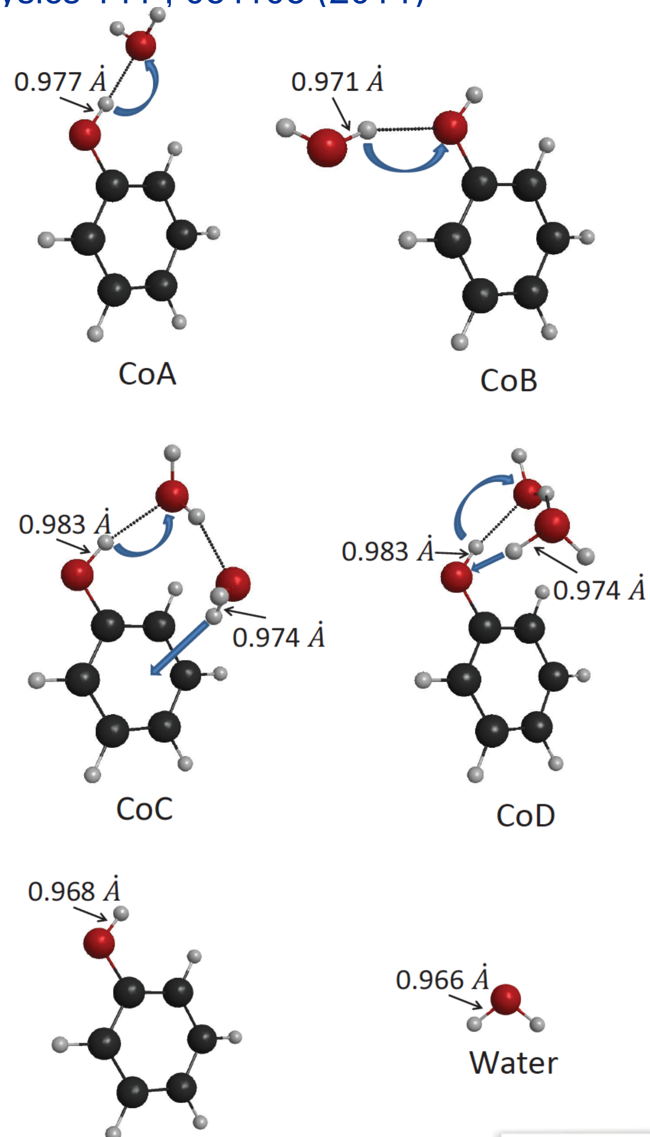
π^* shape resonance for HCOOH at around 1.9 eV.



Electron Collisions with Phenol...H_2O

E. M. de Oliveira, T. C. Freitas , K. Coutinho , M. T. do N. Varella , S. Canuto , M. A. P. Lima and M.H.F Bettega, The Journal of Chemical Physics 141 , 051105 (2014)



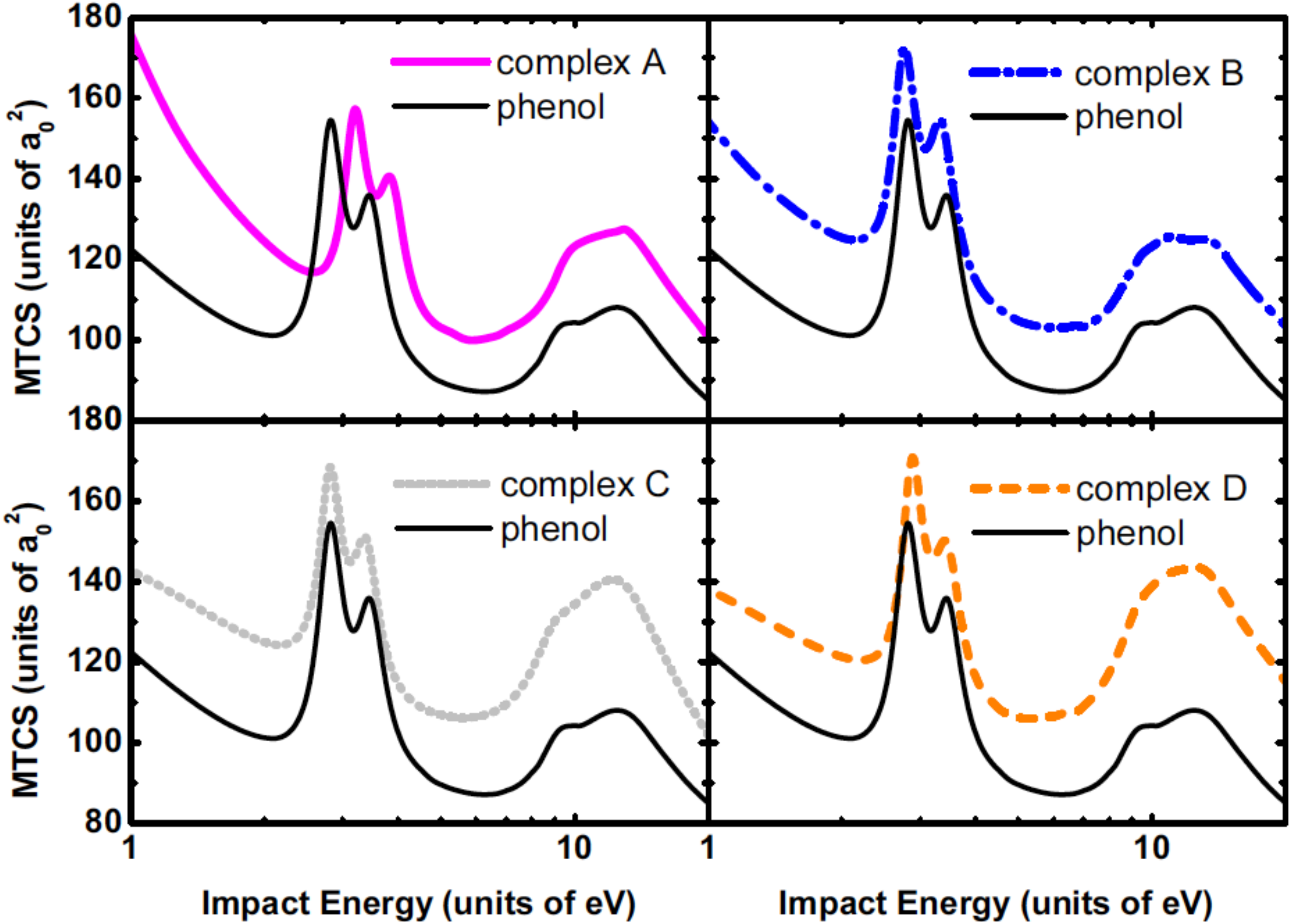


We have studied the microsolvation of Phenol using 4 complexes.

- 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).

In real situations the resonances may change positions due to an overall donor or acceptor effect!

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



How useful are these calculations to a modeler?

ELECTRONIC EXCITATION

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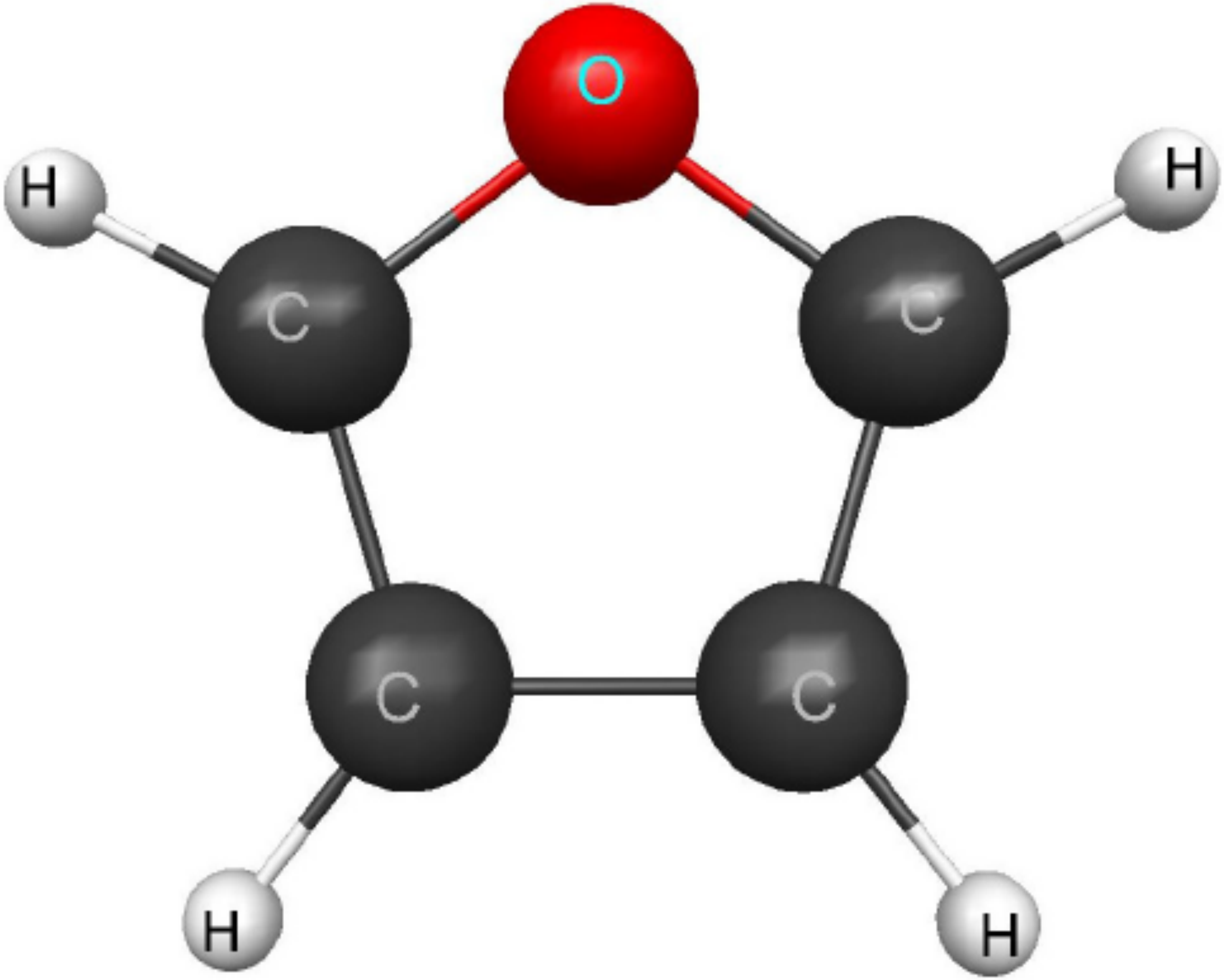
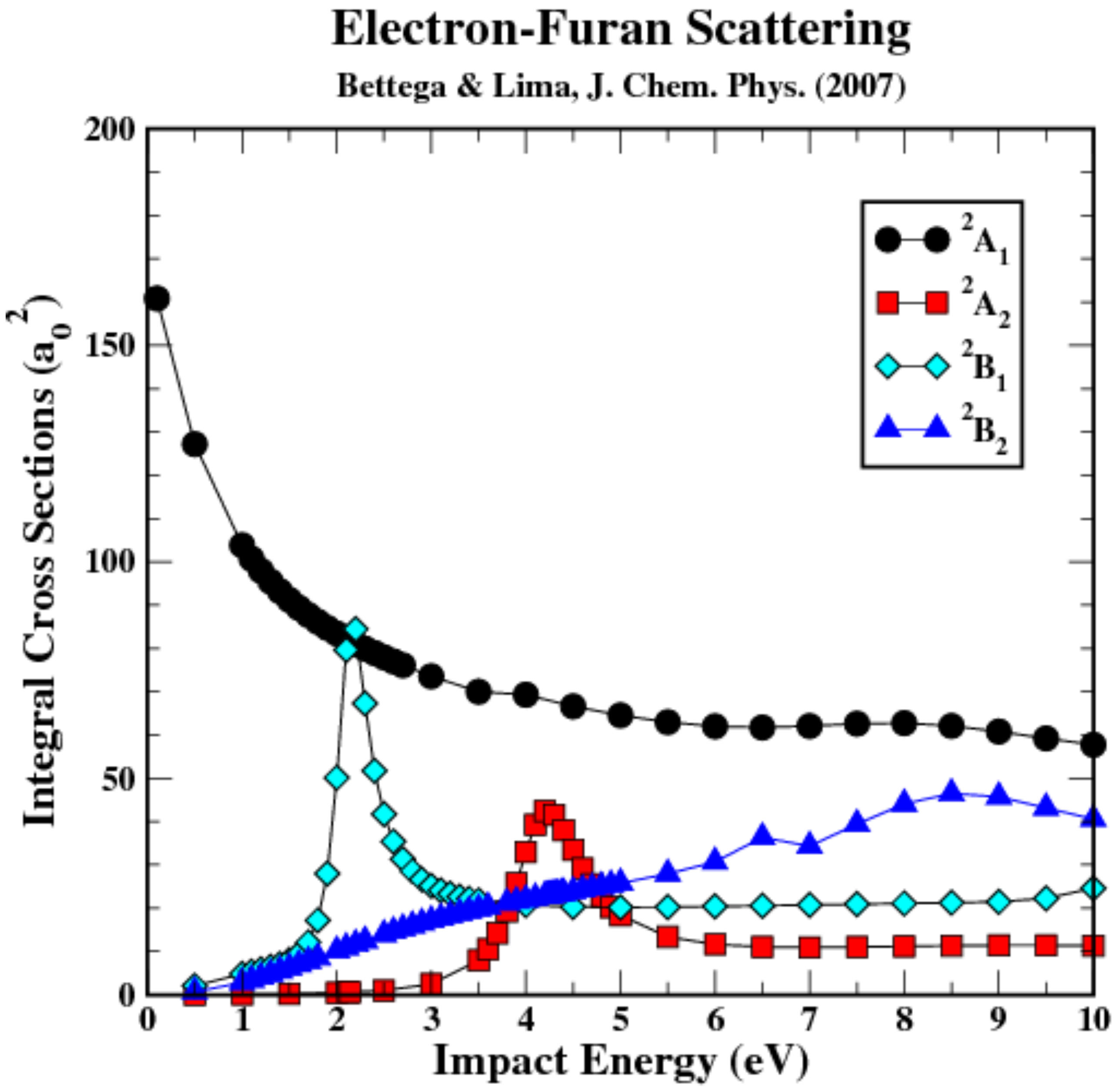
Is it enough just to find the positions and widths of existing resonances?

Electronic excitation of furan by electron impact



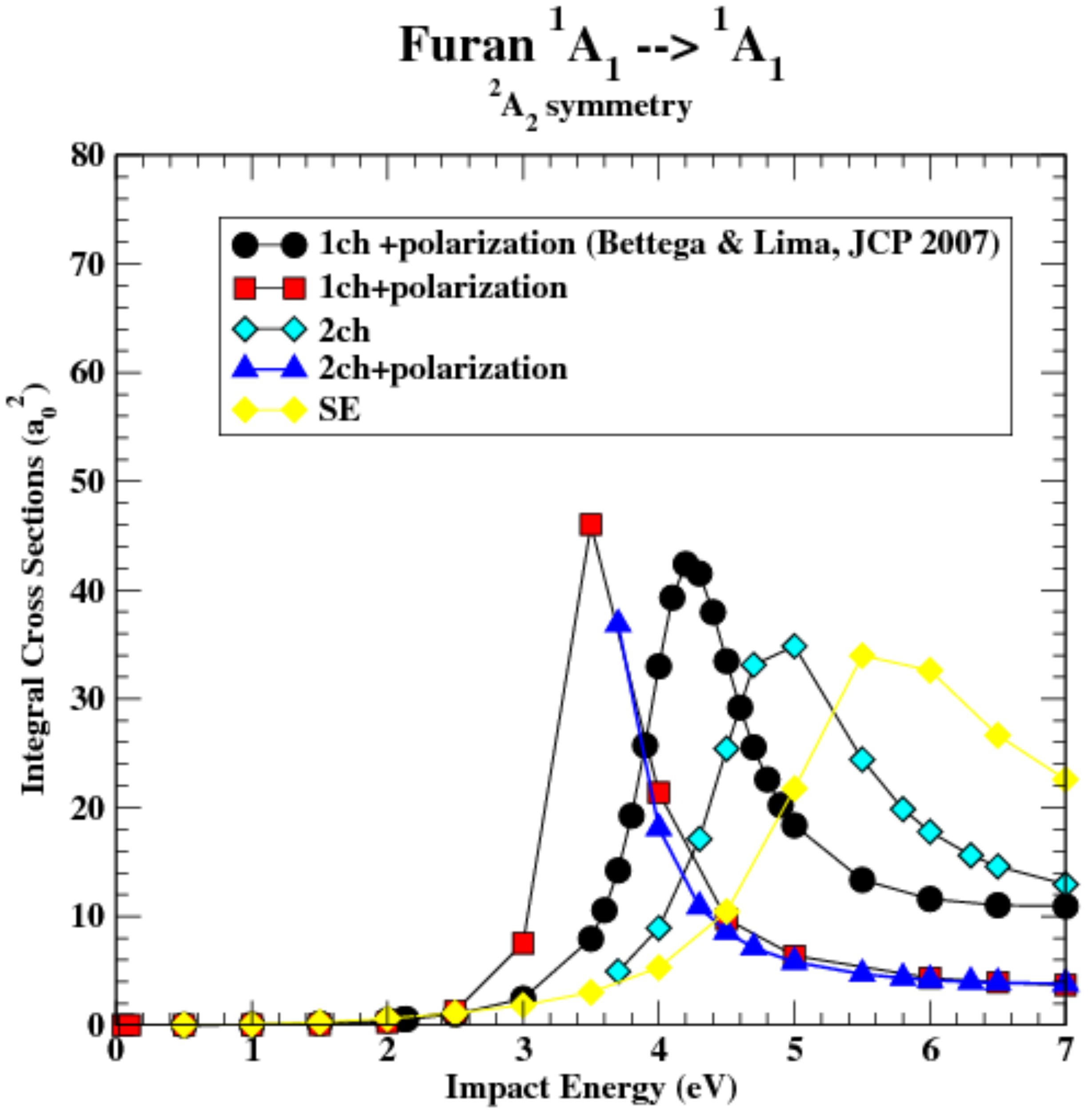
Special attention to low energy triplet states

Furan presents two shape resonances at low impact energies



APS physics

Polarization effects strongly affect the resonance positions



Finding resonance's positions and widths may not be enough!

R. F. da Costa, M. H. F. Bettega, and M. A. P. Lima, *Phys. Rev. A* **77**, 012717-20 (2008).

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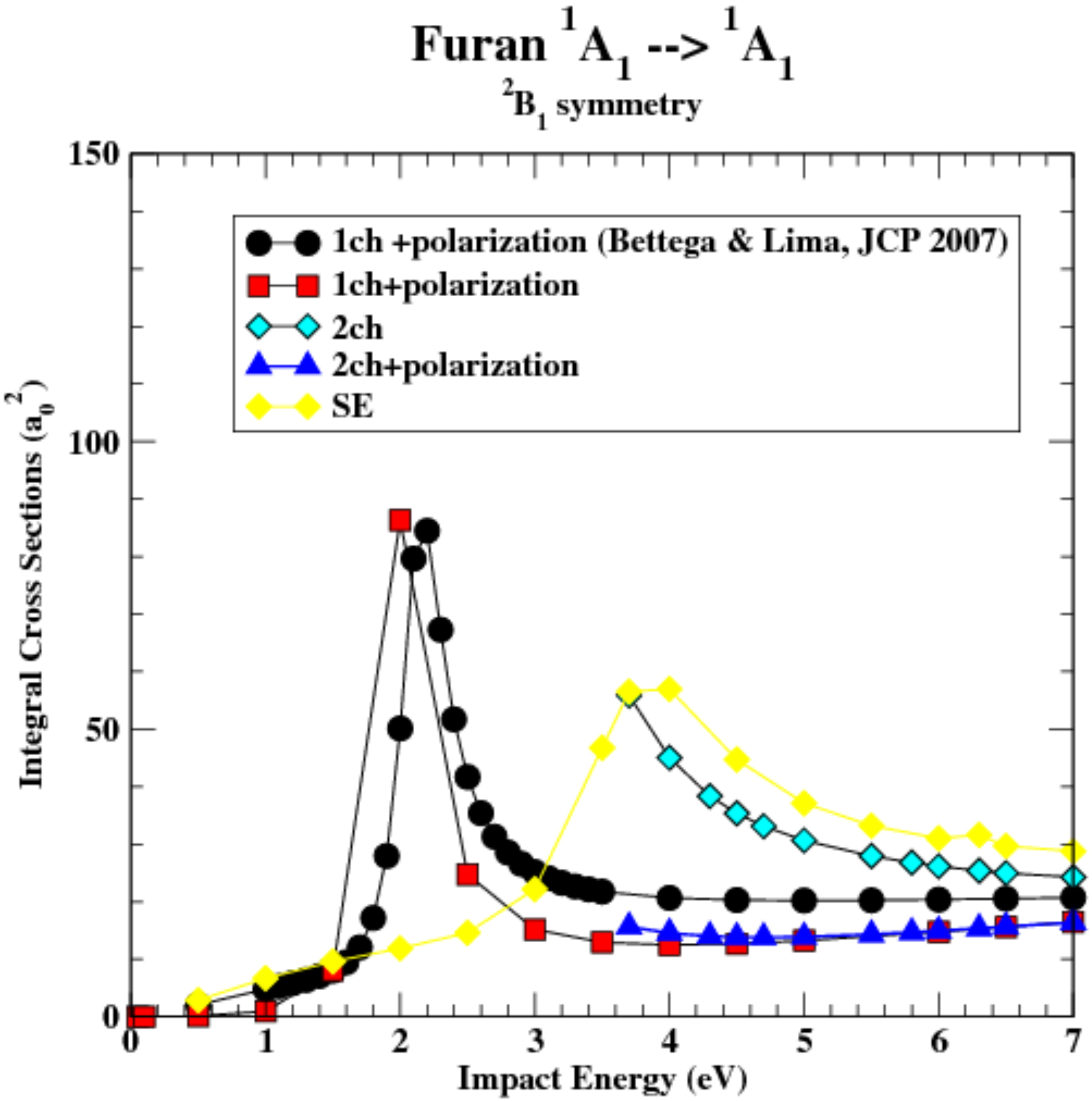
Honolulu

R. F. da Costa, M. H. F. Bettega, and M. A. P. Lima, *Phys. Rev. A* **77**, 012717-20 (2008).

Polarization effects strongly affect the resonance positions



Finding resonance's positions and widths may not be enough!

MAPLima

APS physics

R. F. da Costa, M. H. F. Bettega, and M. A. P. Lima, *Phys. Rev. A* **77**, 012717-20 (2008).

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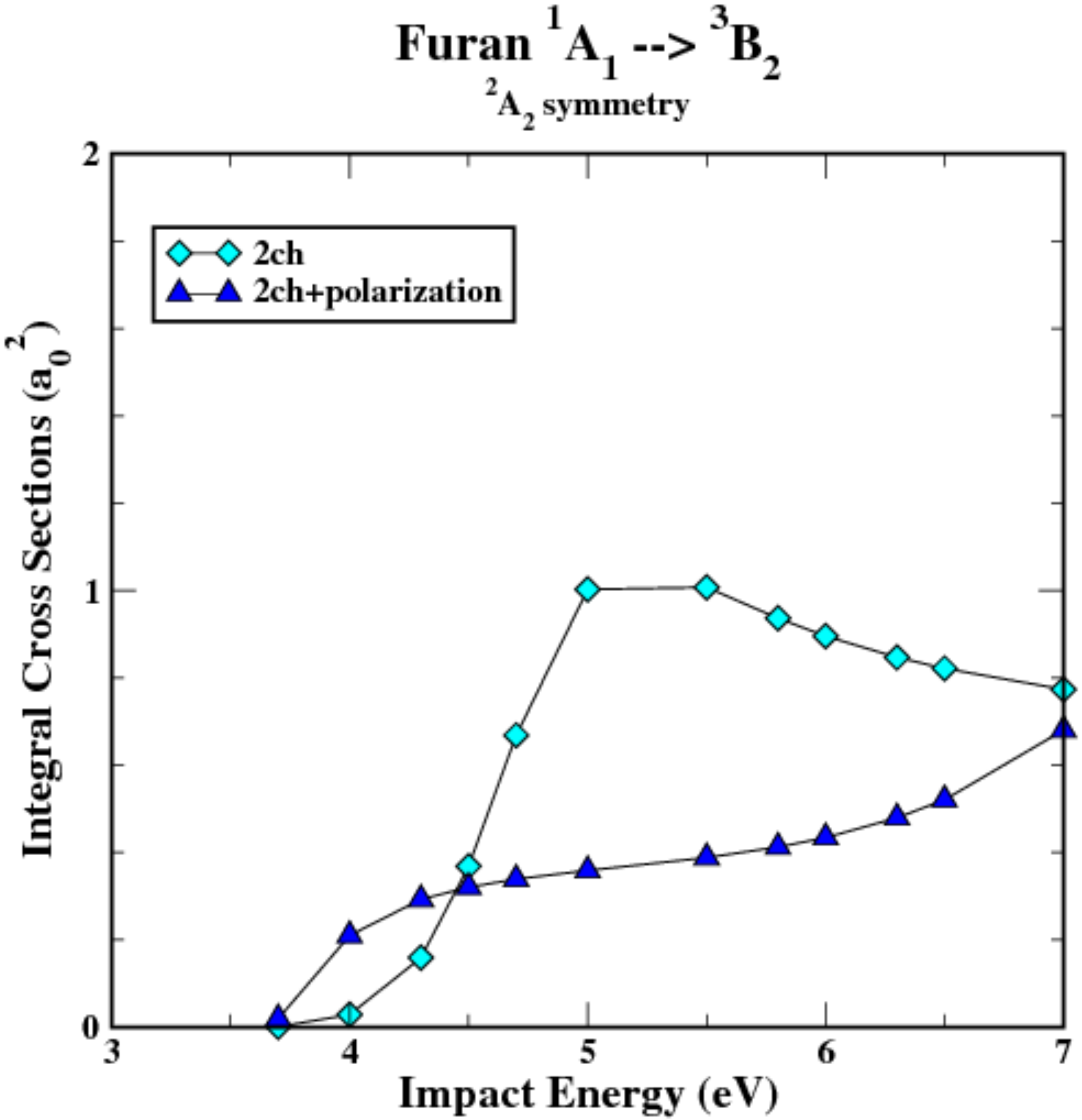
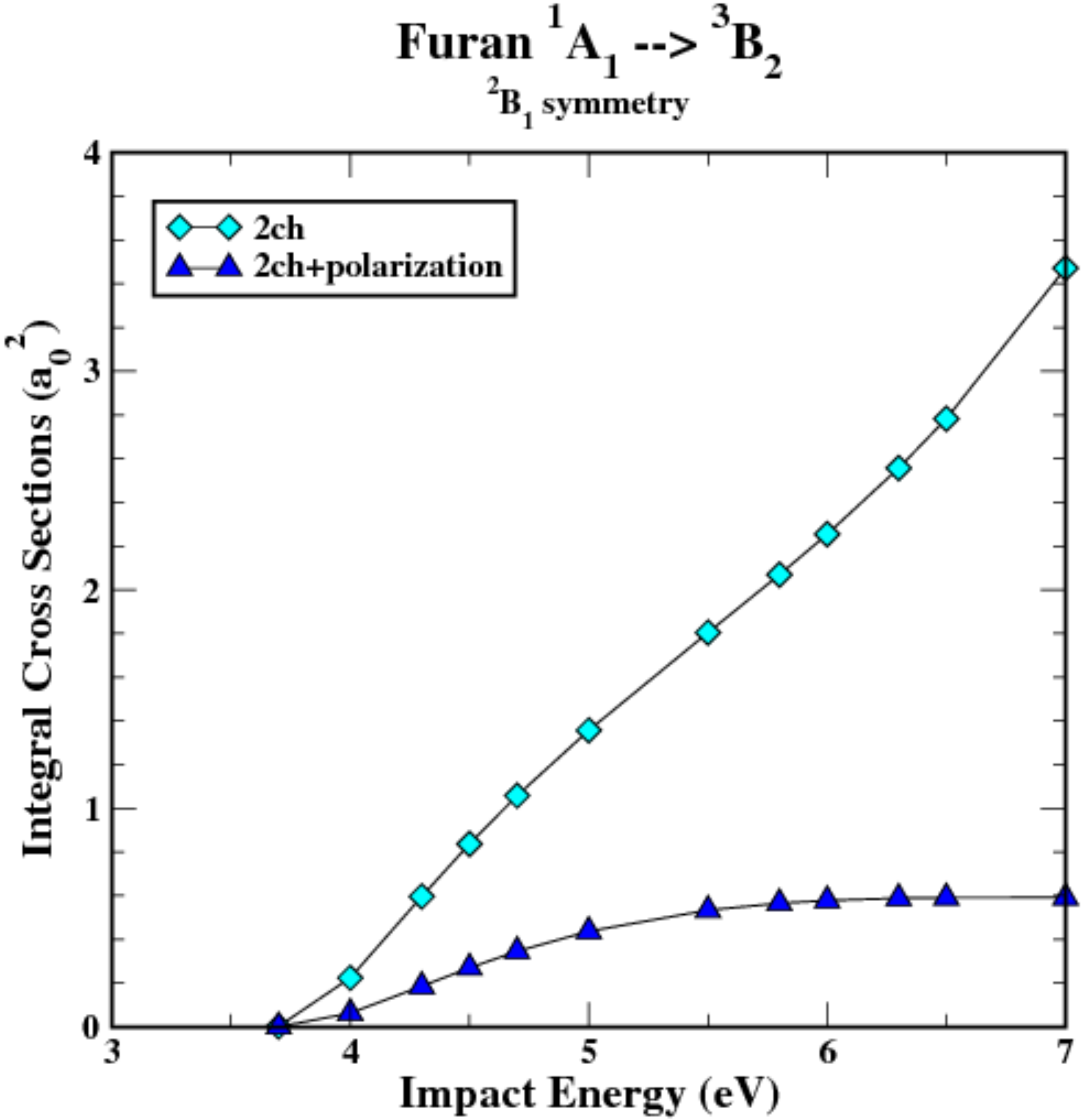
The resonance positions strongly affect the excitation cross sections



How would that affect a plasma modeling?

R. F. da Costa, M. H. F. Bettega, and M. A. P. Lima, *Phys. Rev.A* **77**, 012717-20 (2008).

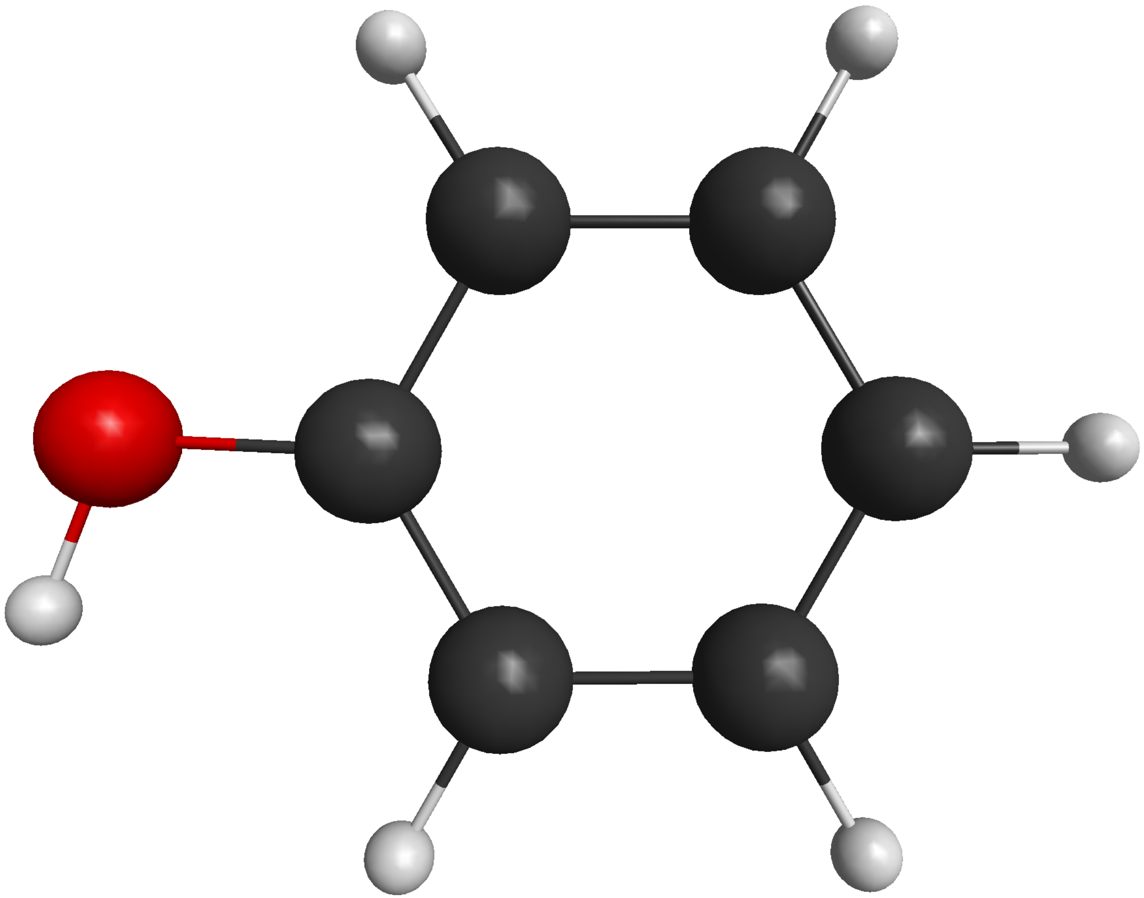
The resonance positions strongly affect the excitation cross sections



How would that affect a plasma modeling?

Electronic excitation of Phenol by electron impact

D. B. Jones, G. B. da Silva, R. F. C. Neves, H.V. Duque, L. Chiari, E. M. de Oliveira, M. C. A. Lopes, R. F. da Costa, M. T. do N. Varella, M. H. F. Bettega, M. A. P. Lima, and M. J. Brunger, *J. Chem. Phys.* **141**, 074314 (2014). First of a series of papers under the Science without Border Program (CNPq/CAPES).



D. B. Jones, G. B. da Silva, R. F. C. Neves, H. V. Duque, L. Chiari, E. M. de Oliveira, M. C. A. Lopes, R. F. da Costa, M. T. do N. Varella, M. H. F. Bettega, M. A. P. Lima, and M. J. Brunger, *J. Chem. Phys.* **141**, 074314 (2014)

074314-4 Jones *et al.* J. Chem. Phys. **141**, 074314 (2014)

e⁻ - Phenol scattering

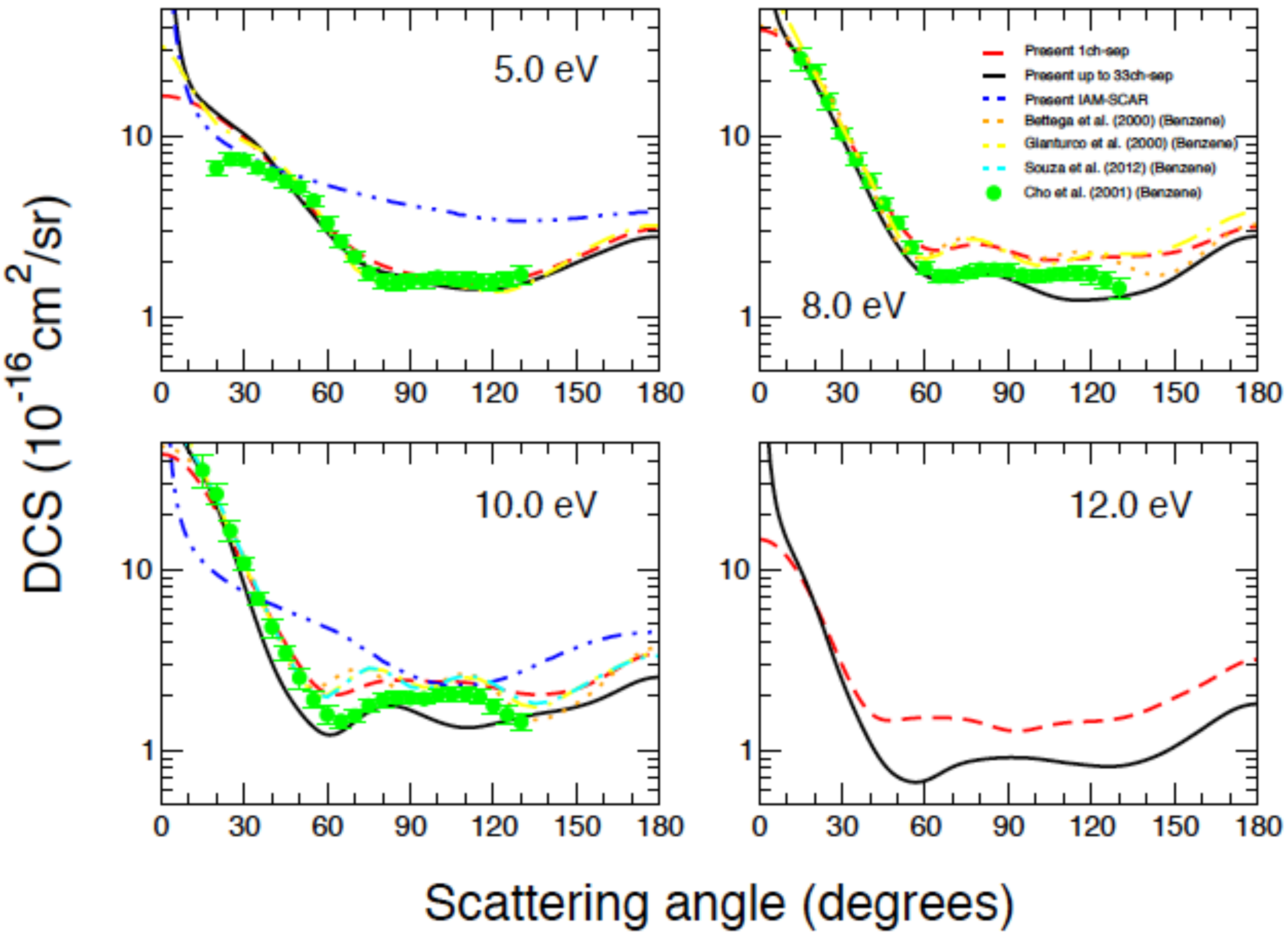
TABLE I. Experimental and calculated excitation energies, assignments, dominant configurations, and optical oscillator strengths (f_0).

			TD-DFT			MOB-SCI		Full-SCI	
Band	Expt. energy (eV)	State	Energy (eV)	Dominant excitation(s)	f_0	Energy (eV)	f_0	Energy (eV)	f_0
I	3.4–4.3	$^3A'$	3.71	$3a''\to5a''$; $4a''\to6a''$	0	3.57	0	3.29	0
		$^3A'$	4.10	$4a''\to5a''$	0	4.73	0	4.49	0
II	4.3–5.4	$^3A'$	4.53	$3a''\to5a''$; $4a''\to6a''$	0	4.90	0	4.78	0
		$^1A'$	4.99	$3a''\to6a''$; $4a''\to5a''$	0.0312	6.09	0.0248	5.82	0.0381
		$^3A''$	5.06	$4a''\to22a'$	0	6.16	0	5.94	0
		$^1A''$	5.13	$4a''\to22a'$	0.0001	6.21	0.0001	6.06	0.0001
		$^3A'$	5.30	$3a''\to6a''$	0	6.03	0	5.73	0
III	5.4–6.3	$^3A''$	5.53	$4a''\to23a'$	0	6.78	0	6.53	0
		$^1A''$	5.57	$4a''\to23a'$	0.0034	6.86	0.0274	6.68	0.0177
		$^1A'$	5.76	$3a''\to5a''$; $4a''\to6a''$	0.0328	6.80	0.0031	6.12	0.0025
		$^3A''$	5.90	$3a''\to22a'$; $4a''\to24a'$	0	6.92	0	6.73	0
		$^1A''$	5.92	$4a''\to24a'$	0				
		$^3A''$	5.95	$3a''\to22a''$; $4a''\to24a'$	0				
		$^1A''$	5.98	$3a''\to22a'$	0.0021	6.99	0	6.86	0.0020
		$^3A''$	6.27	$4a''\to25a'$	0				
IV	6.3–7.3	$^1A''$	6.31	$4a''\to25a'$	0.0115				
		$^3A''$	6.32	$3a''\to23a'$	0				
		$^1A''$	6.35	$3a''\to23a'$	0.0010				
		$^3A''$	6.52	$4a''\to26a'$	0				
		$^1A''$	6.54	$4a''\to26a'$	0				
		$^3A''$	6.63	$3a''\to24a'$	0				
		$^1A'$	6.66	$3a''\to6a''$	0.3744				
		$^1A''$	6.66	$3a''\to24a'$	0.0202				
		$^1A'$	6.71	$3a''\to5a''$; $4a''\to6a''$	0.5827				
		$^3A''$	6.84	$4a''\to27a'$; $4a''\to28a'$	0				
		$^3A'$	6.85	$2a''\to5a''$	0				
		$^3A'$	6.93	$4a''\to7a''$	0				
		$^1A''$	6.93	$4a''\to27a'$; $4a''\to28a'$	0.0009				
		$^1A'$	7.01	$4a''\to7a''$	0.0148				
		$^3A''$	7.07	$3a''\to25a'$	0				
		$^1A''$	7.08	$3a''\to25a'$	0				
		$^3A'$	7.11	$2a''\to6a''$	0				
		$^3A''$	7.19	$4a''\to27a'$; $4a''\to28a'$	0				
		$^1A''$	7.22	$4a''\to27a'$; $4a''\to28a'$	0.0005				
		$^3A''$	7.27	$21a'\to5a''$	0				
		$^3A''$	7.29	$3a''\to26a'$	0				
V	7.3–8.6	$^1A''$	7.32	$3a''\to26a'$	0.0002				
		$^1A''$	7.57	$21a'\to5a''$	0.0043				
		$^3A''$	7.58	$4a''\to29a'$	0				
		$^3A''$	7.59	$3a''\to27a'$; $3a''\to28a'$	0				

No state-by-state resolution. Our experimental resolution is by bands of electronic states

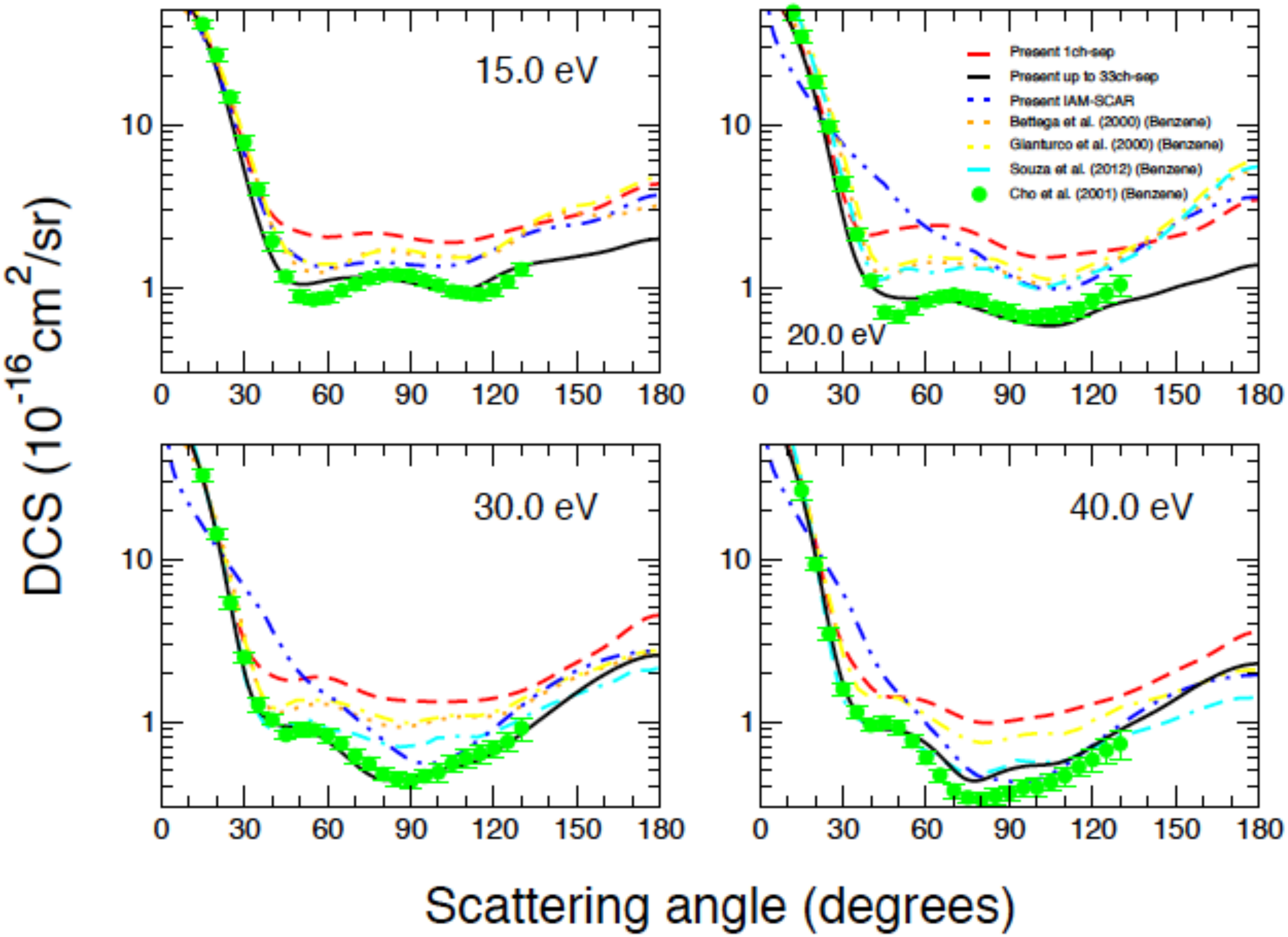
Our scattering calculations have 5 singlets and 7 triplets below 7eV in good agreement with the full single configuration interaction. We also included 20 additional pseudo states as possible open channels (a total of 33 channels)

Multichannel coupling on electron-Phenol scattering: Effects on the Elastic channel



R. F. da Costa, E. M. de Oliveira, M. H. F. Bettega, M. T. do N. Varella, D. B. Jones, M. J. Brunger, F. Blanco, R. Colmenares, P. Limão-Vieira, G. García, and M. A. P. Lima, *J. Chem. Phys.* **142**, 104304 (2015).

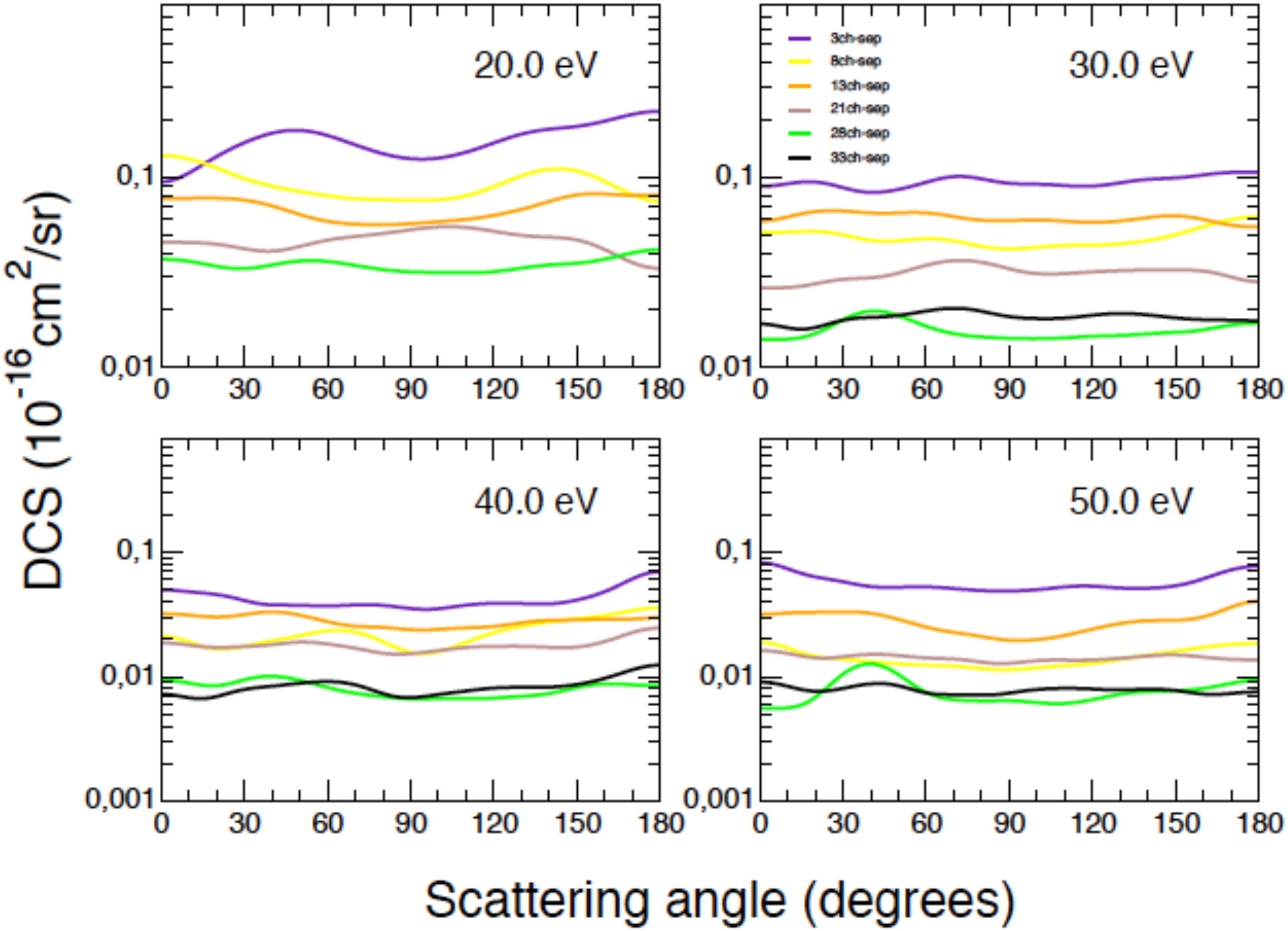
Multichannel coupling on electron-Phenol scattering: Effects on the Elastic channel



Flux competition is a important effect. As we open more channels the flux to a particular state decreases.

R. F. da Costa, E. M. de Oliveira, M. H. F. Bettega, M. T. do N. Varella, D. B. Jones, M. J. Brunger, F. Blanco, R. Colmenares, P. Limão-Vieira, G. Garcia, and M.A. P. Lima, *J. Chem. Phys.* **142**, 104304 (2015).

Multichannel coupling on electron-Phenol scattering: Effects on the first triplet state channel



Flux competition is a important effect. As we open more channels the flux to a particular state decreases.

It reminds a classical picture of a river blocked by gates. As you open more gates the flux through all of them decreases.

R. F. da Costa, E. M. de Oliveira, M. H. F. Bettega, M. T. do N. Varella, D. B. Jones, M. J. Brunger, F. Blanco, R. Colmenares, P. Limão-Vieira, G. García, and M. A. P. Lima, *J. Chem. Phys.* **142**, 104304 (2015).

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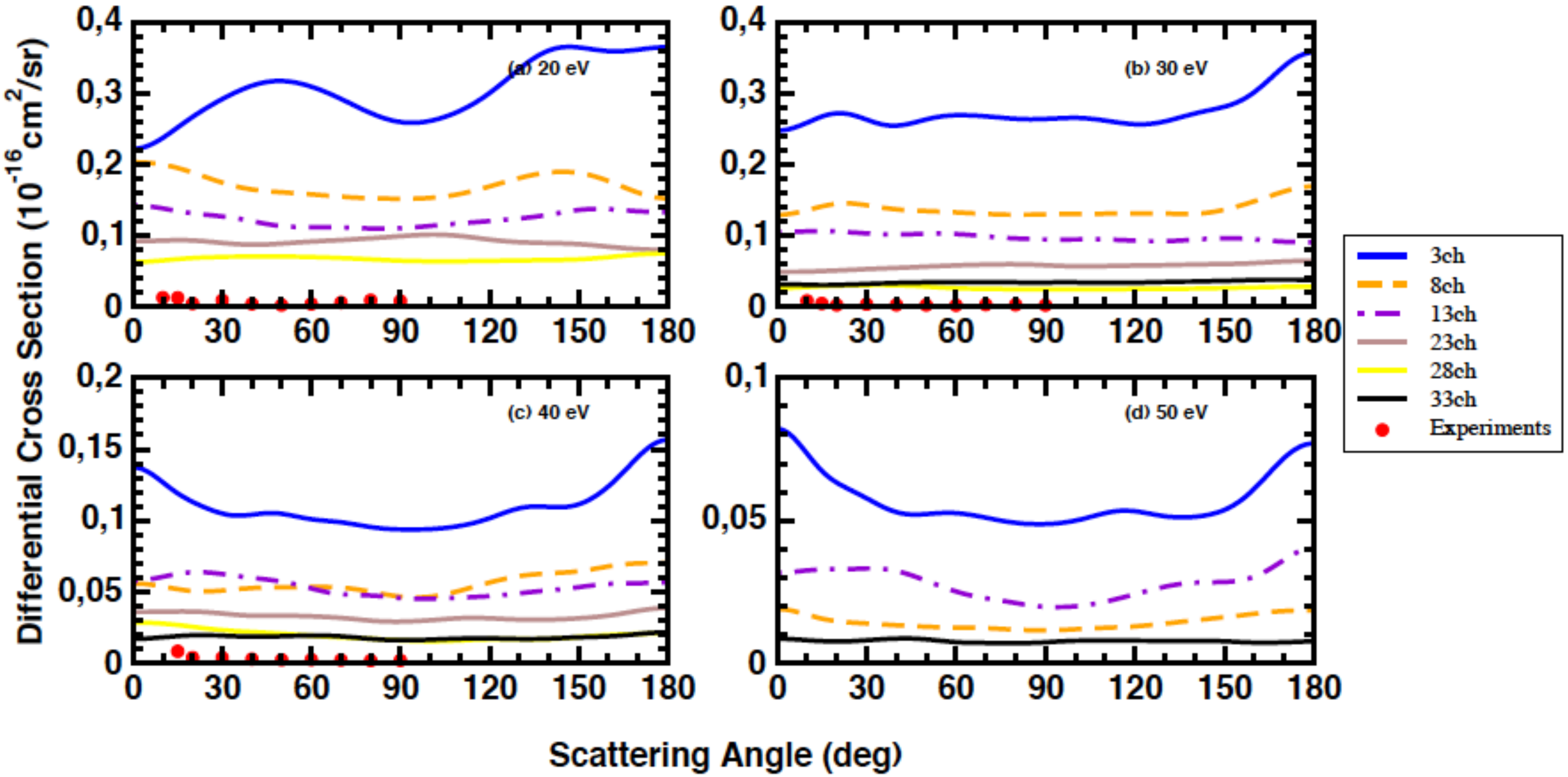
Flux competion is also present in the inelastic process

R. F. C. Neves, D. B. Jones, M. C. A. Lopes, K. L. Nixon, G. B. Da Silva, H. V. Duque, E. M. de Oliveira, R. F. da Costa, M. T. do N. Varella, M. H. F. Bettega, M. A. P. Lima, K. Ratnavelu, G. García, and M. J. Brunger, *J. Chem. Phys.* **142**, 104305 (2015).

Phenol: electronic excitation of Band I



Still a factor of 3-4 from experiments. How would that affect modeling?

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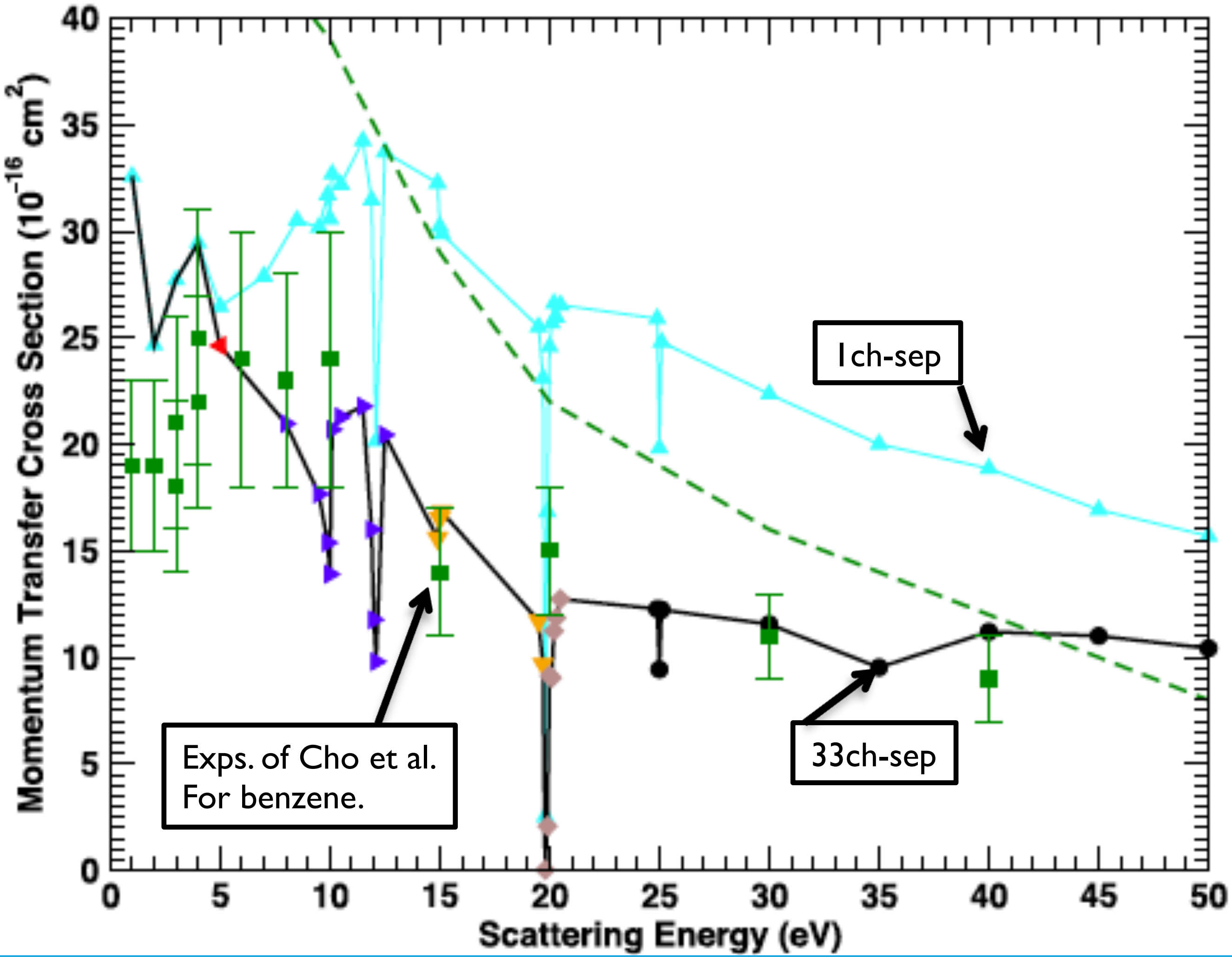
Multichannel effects on the elastic momentum transfer cross sections for electron-phenol scattering



How this big change, caused by multichannel effects, in the MTCS would affect modeling?

R. F. da Costa, E. M. de Oliveira, M. H. F. Bettega, M. T. do N. Varella, D. B. Jones, M. J. Brunger, F. Blanco, R. Colmenares, P. Limão-Vieira, G. Garcia, and M. A. P. Lima, *J. Chem. Phys.* **142**, 104304 (2015).

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R. F. da Costa, E. M. de Oliveira, M. H. F. Bettega, M.T. do N.Varella, D. B. Jones, M. J. Brunger, F. Blanco, R. Colmenares, P. Limão-Vieira, G. García, and M.A. P. Lima, *J. Chem. Phys.* **142**, 104304 (2015).

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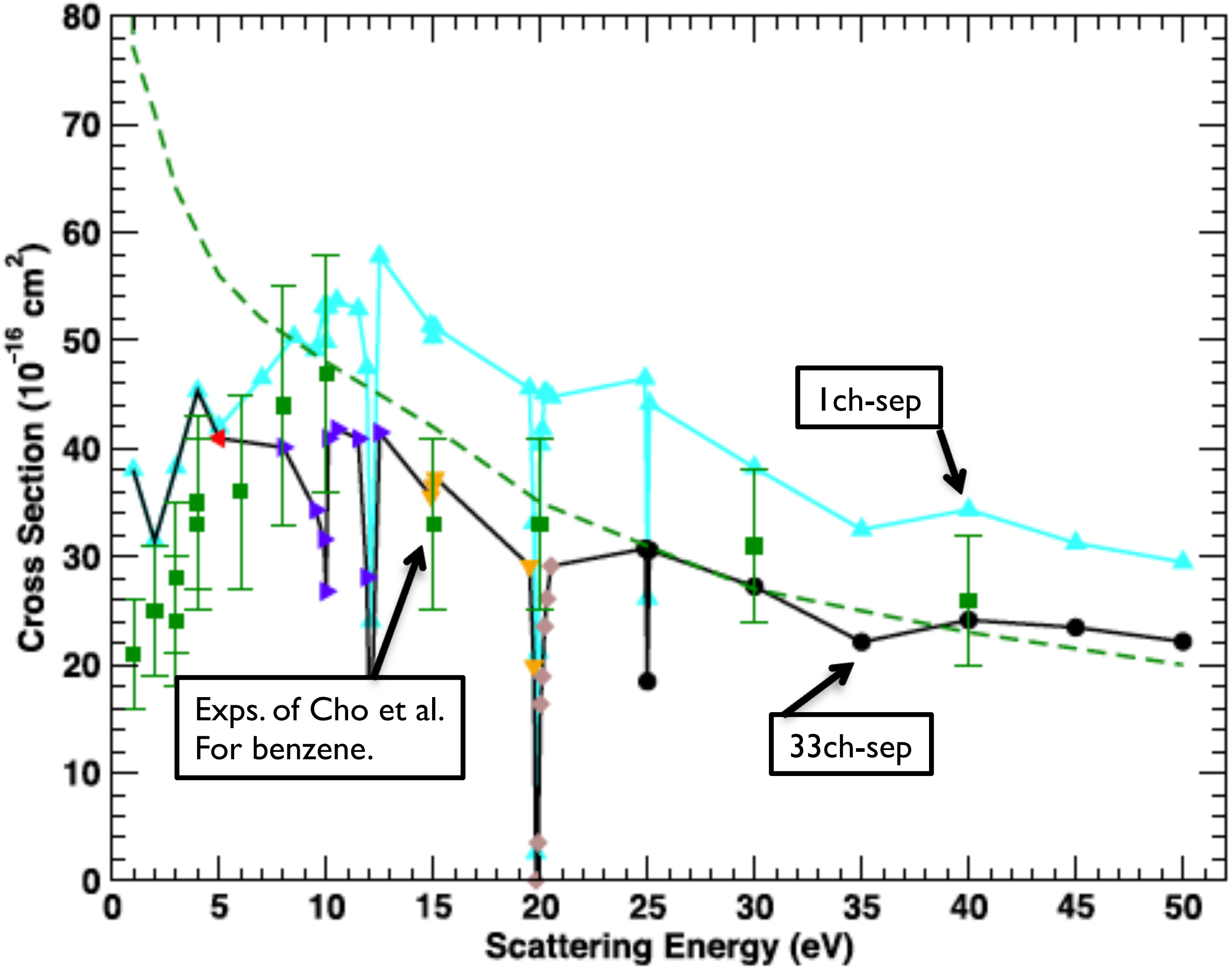
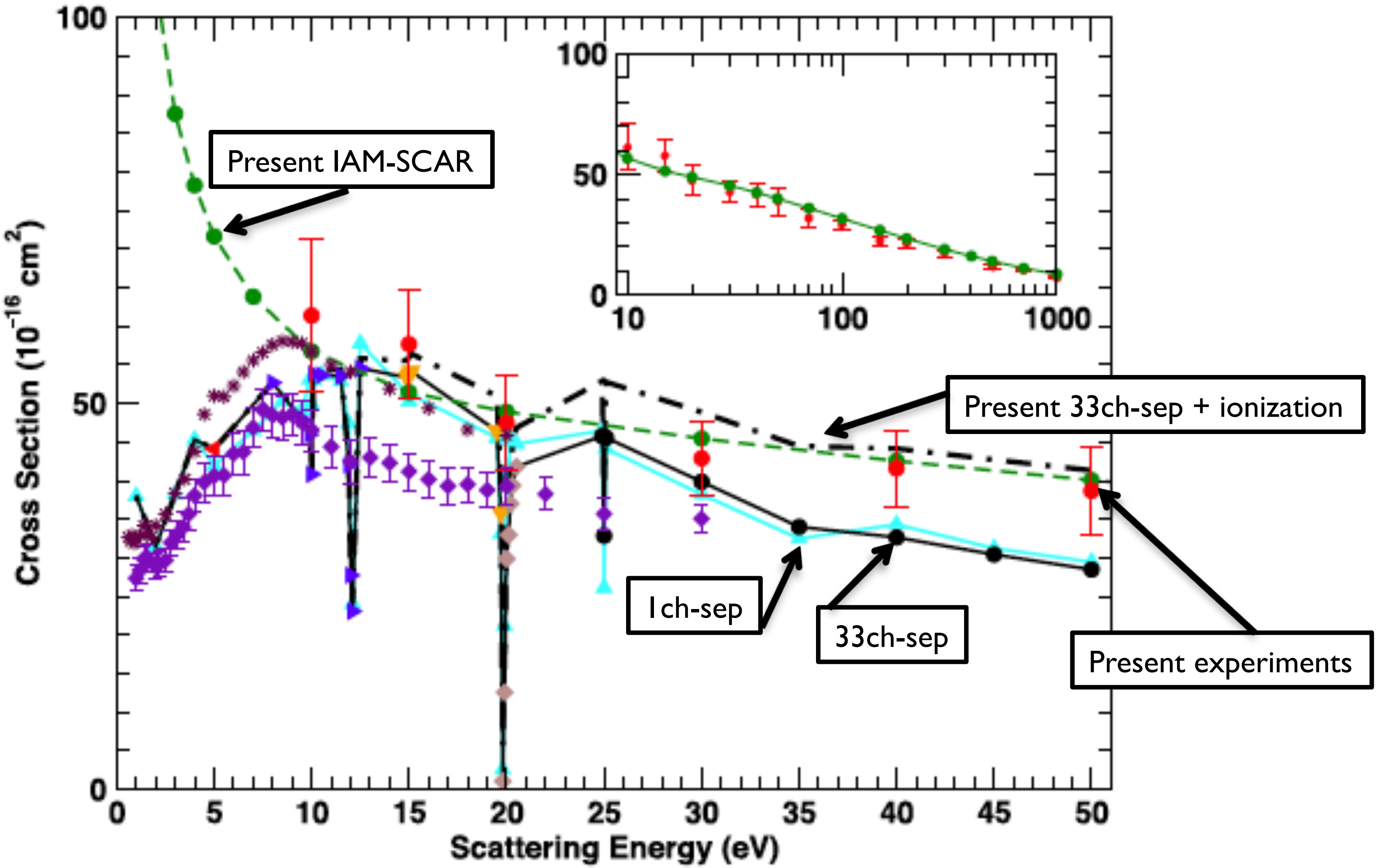
Multichannel effects on the elastic integral cross sections for electron-phenol scattering



How this big change, caused by multichannel effects, in the ICS would affect modeling?

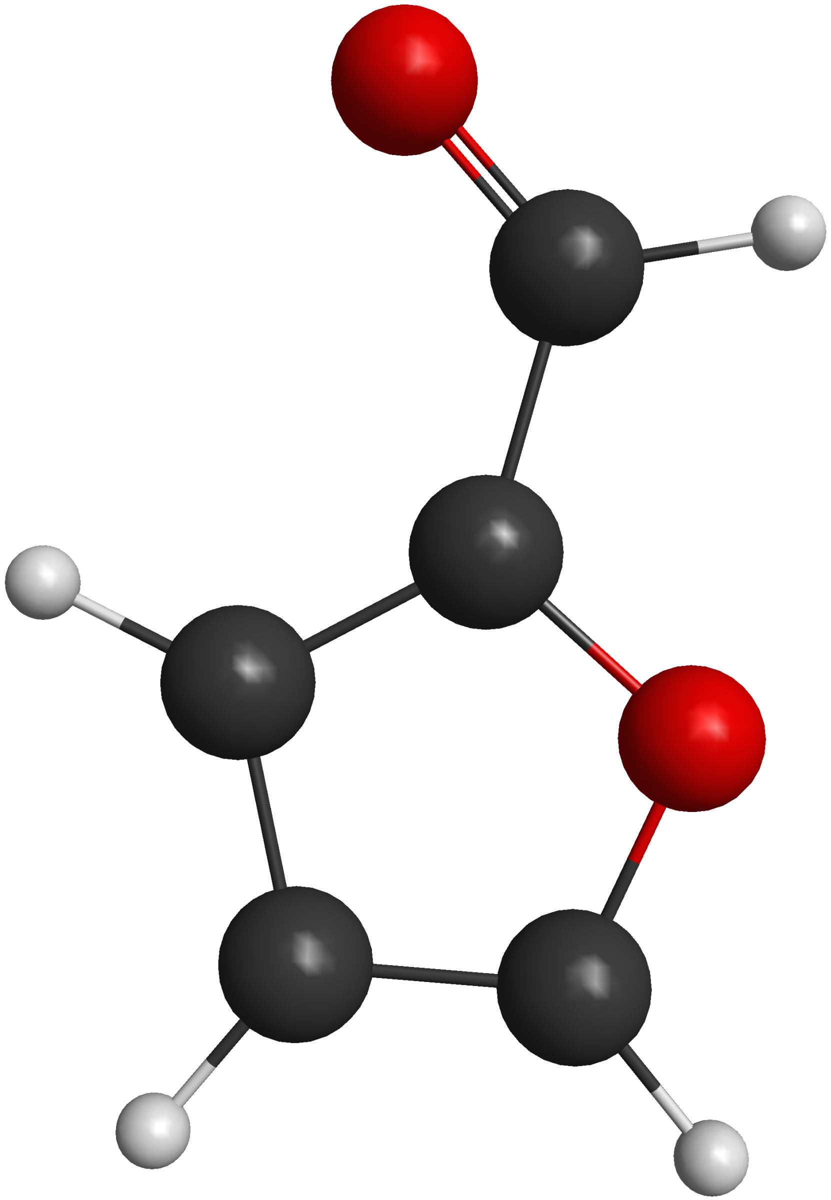
Multichannel effects on total cross sections for electron-phenol scattering



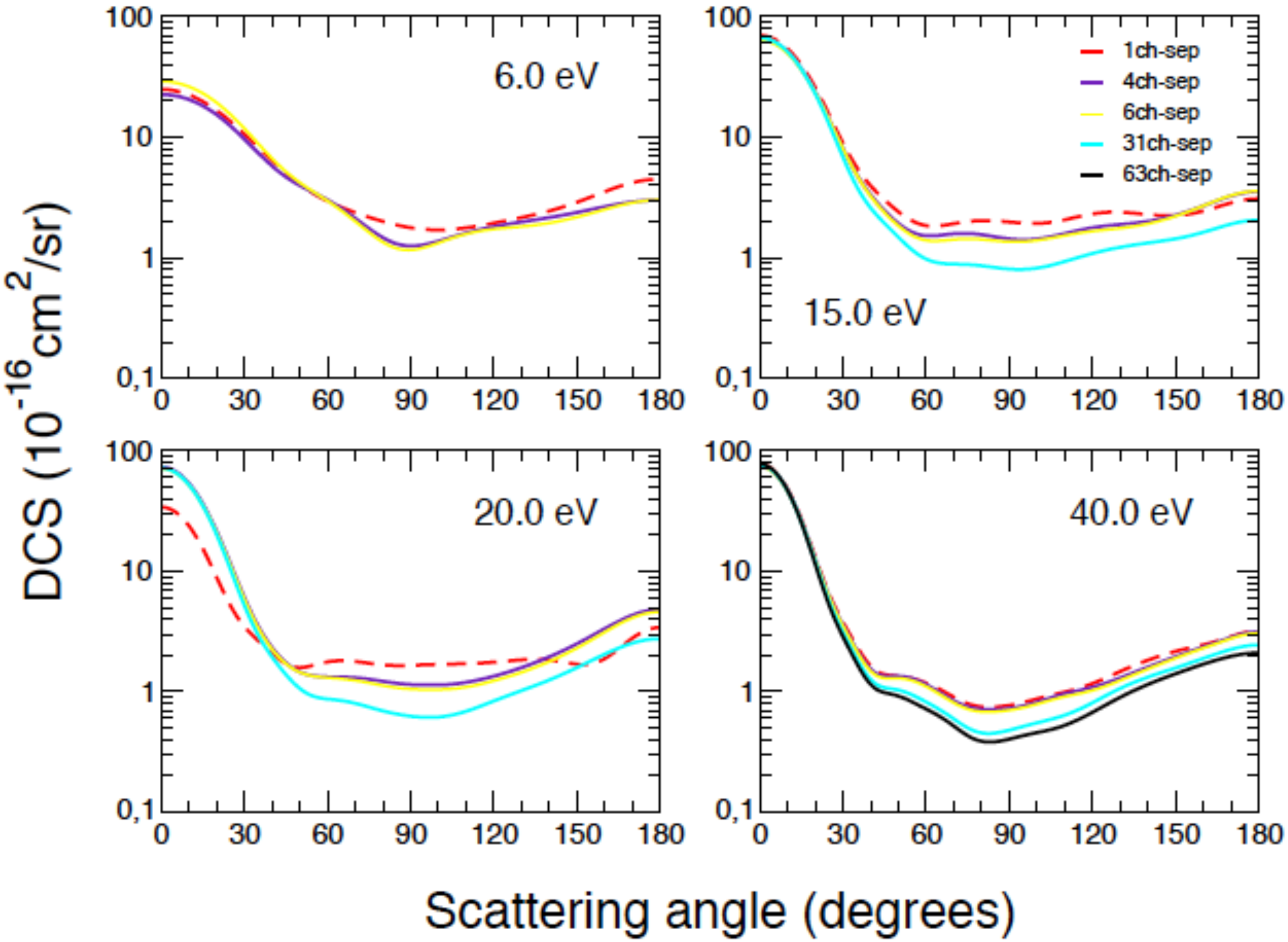
Note that the TCS in the 1ch-sep approximation is similar to the 33ch-sep case. This supports the flux competition picture.

R. F. da Costa, E. M. de Oliveira, M. H. F. Bettega, M. T. do N. Varella, D. B. Jones, M. J. Brunger, F. Blanco, R. Colmenares, P. Limão-Vieira, G. García, and M. A. P. Lima, *J. Chem. Phys.* **142**, 104304 (2015).

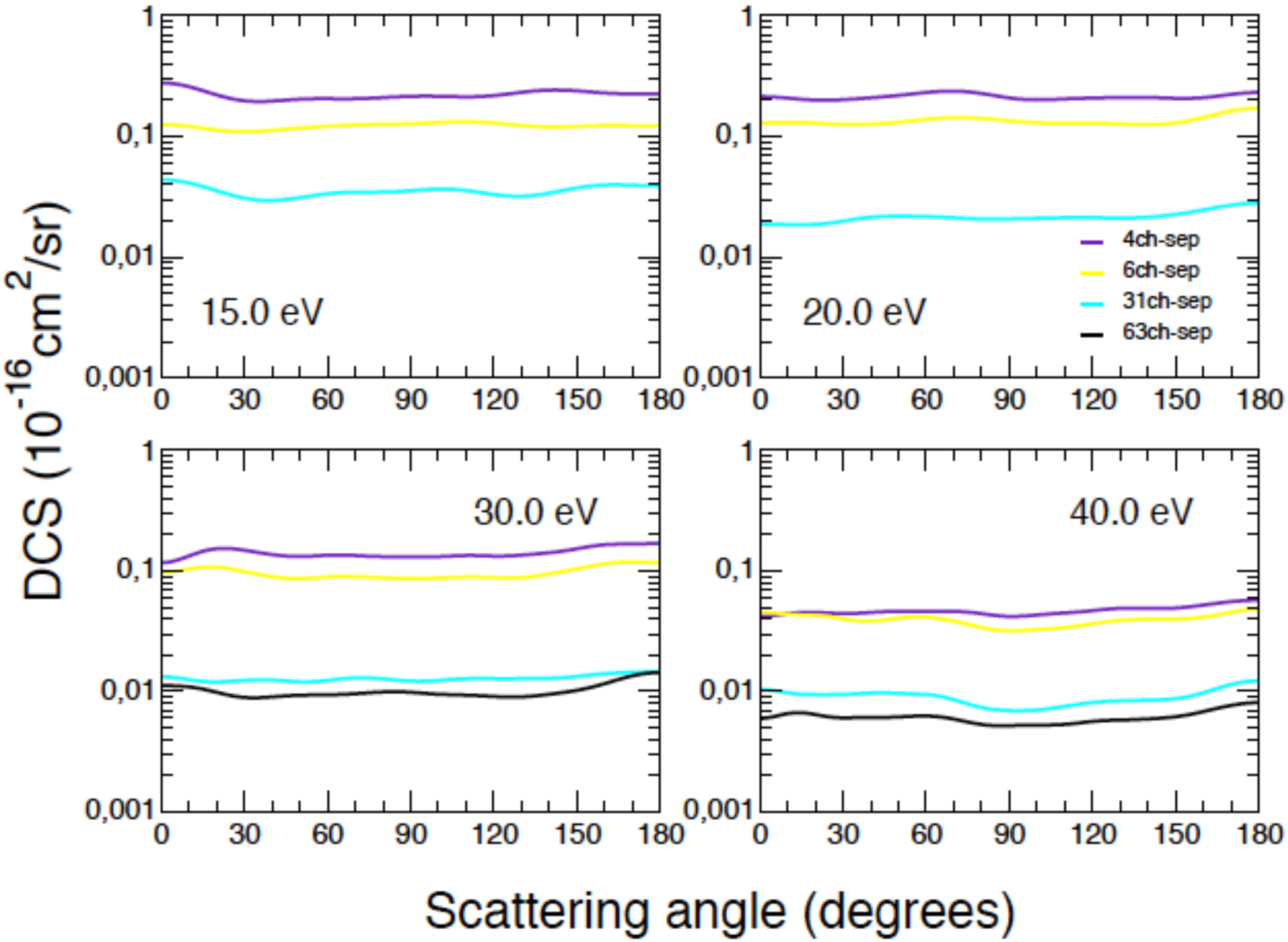
Electronic excitation of furfural by electron impact



Electronic excitation of furfural by electron impact: Effects on the Elastic channel



Electronic excitation of furfural by electron impact: Effects on the first triplet state channel



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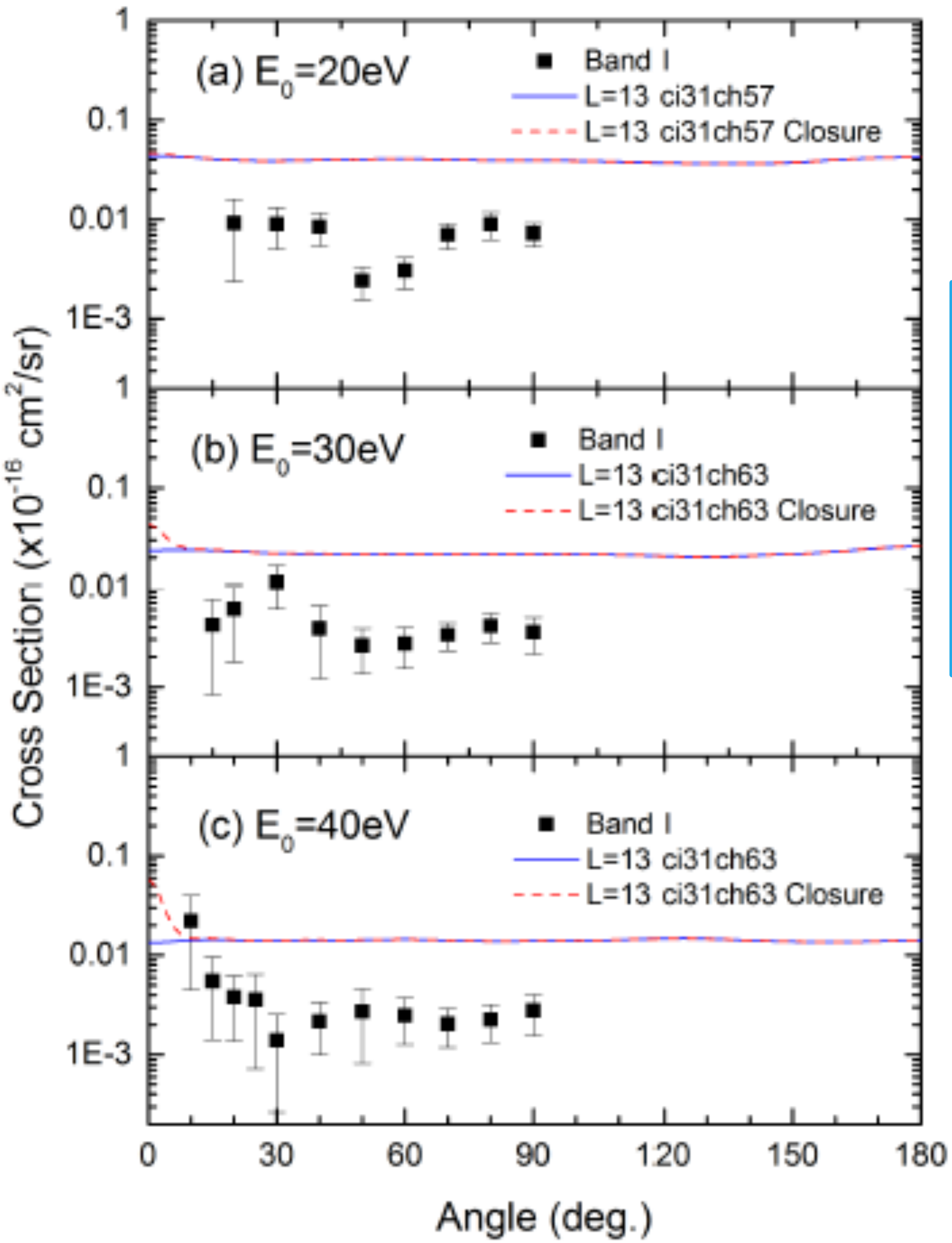
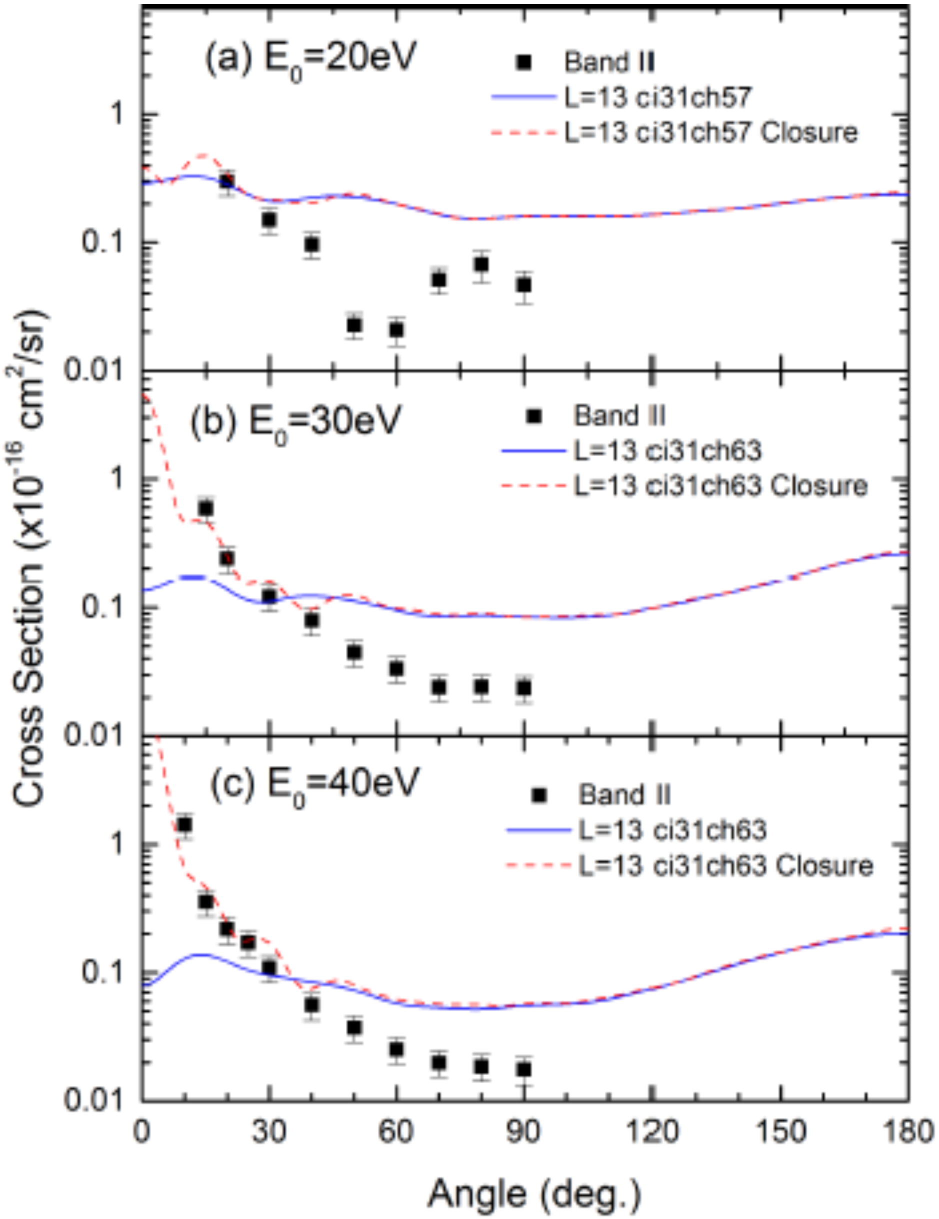
Electronic excitation of Band I of furfural by electron impact:



A factor of 3 difference between theory and experiments. Is it good?

Electronic excitation of Band II of furfural by electron impact:



The DCS at lower angles is dominated by the 1st Born approximation (which may work fine). Higher angles is a factor of 3 to 5 different. Is it good?

CONCLUSION

APS physics

We (from the basic science community on electron-molecule scattering) justify our research on very important and (in some cases) very profitable applications. We have to work closer to plasma modelers in order to assess the quality and importance of our data (theory and experiment).

Thank you very much for your attention

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

All the authors of the papers presented here are co-authors of this presentation

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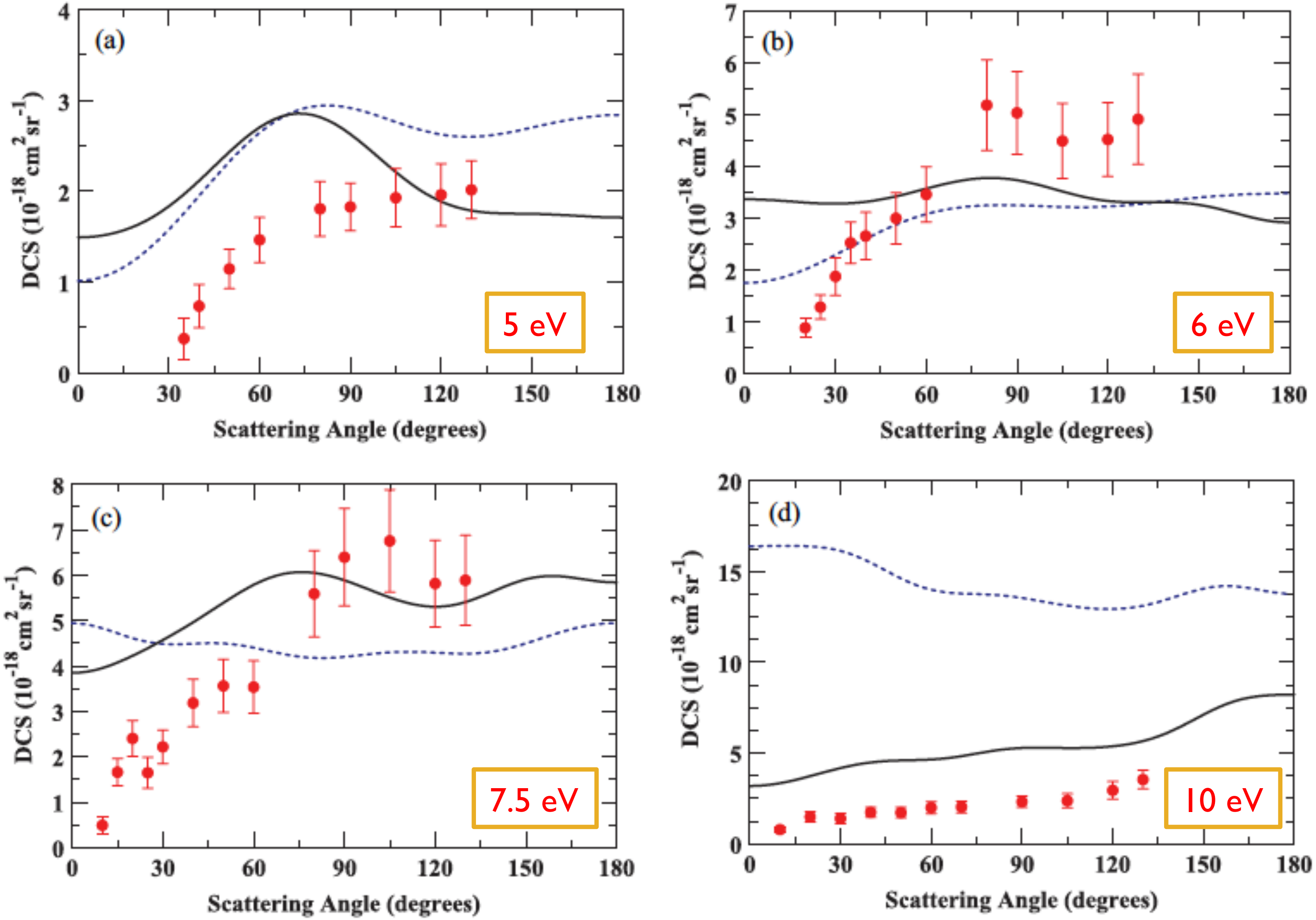
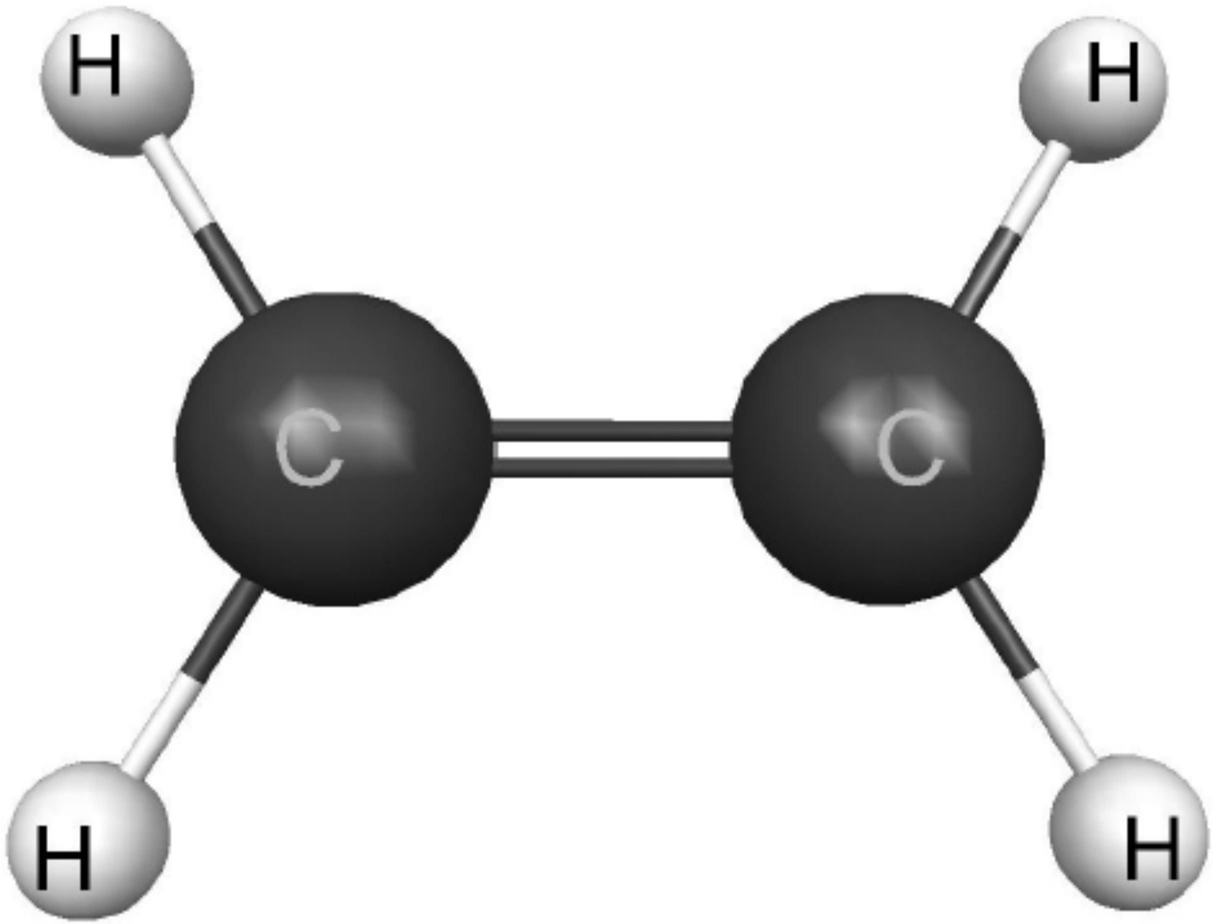
Electronic excitation cross sections of the 1st triplet state of furan



R. F. da Costa, M. H. F. Bettega, and M.A. P. Lima, M. C.A. Lopes, L.R. Hargreaves, G. Serna, M.A. Khakoo, *Phys. Rev.A* **85**, 062706 (2012).

APS physics

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



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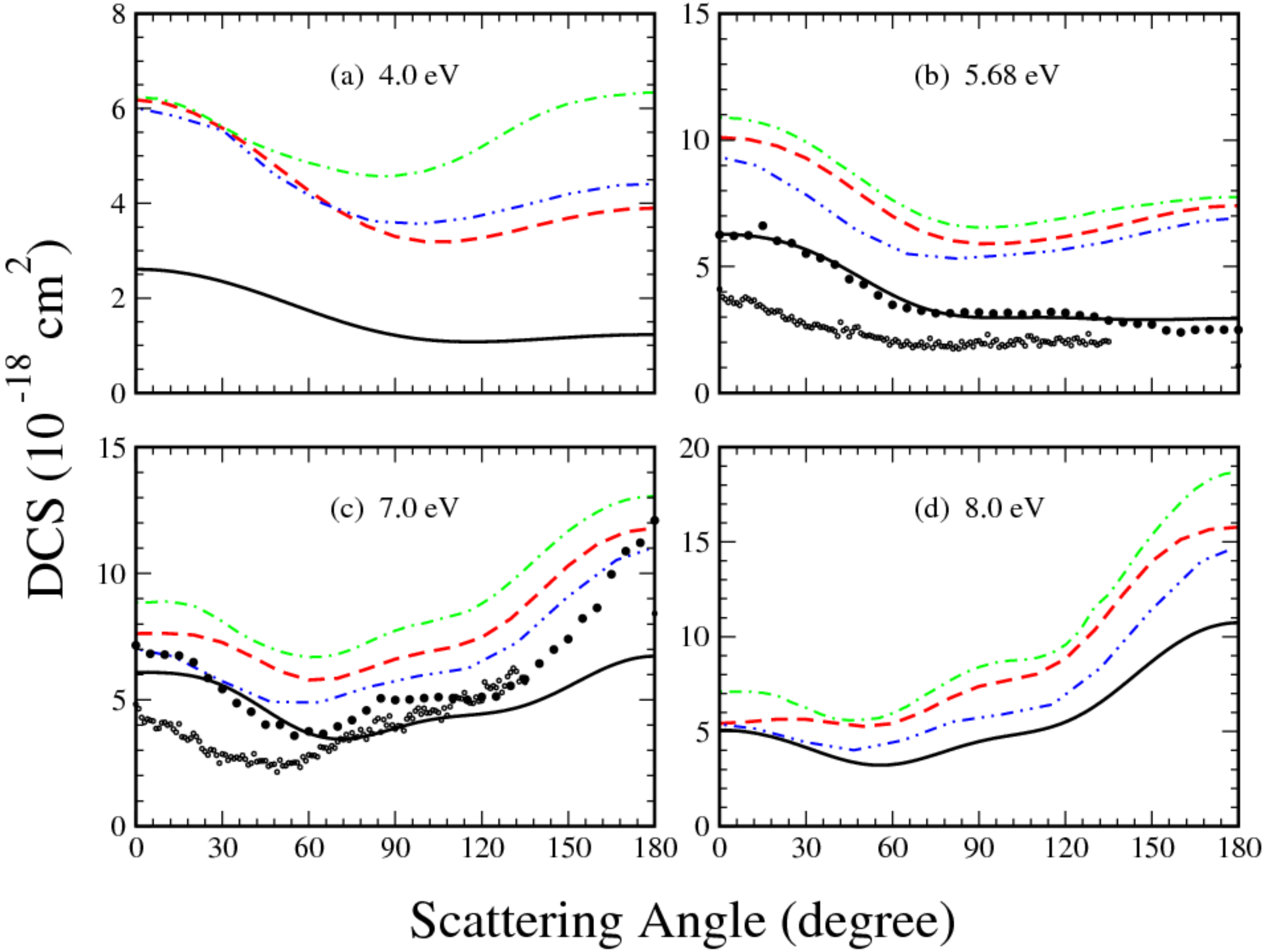
Electronic excitation of ã $^3B_{1u}$ state of C_2H_4 by electron impact



Color lines are 2-channel (close-coupling) results.

Black line are proper balanced n-channel coupling plus polarization effects.

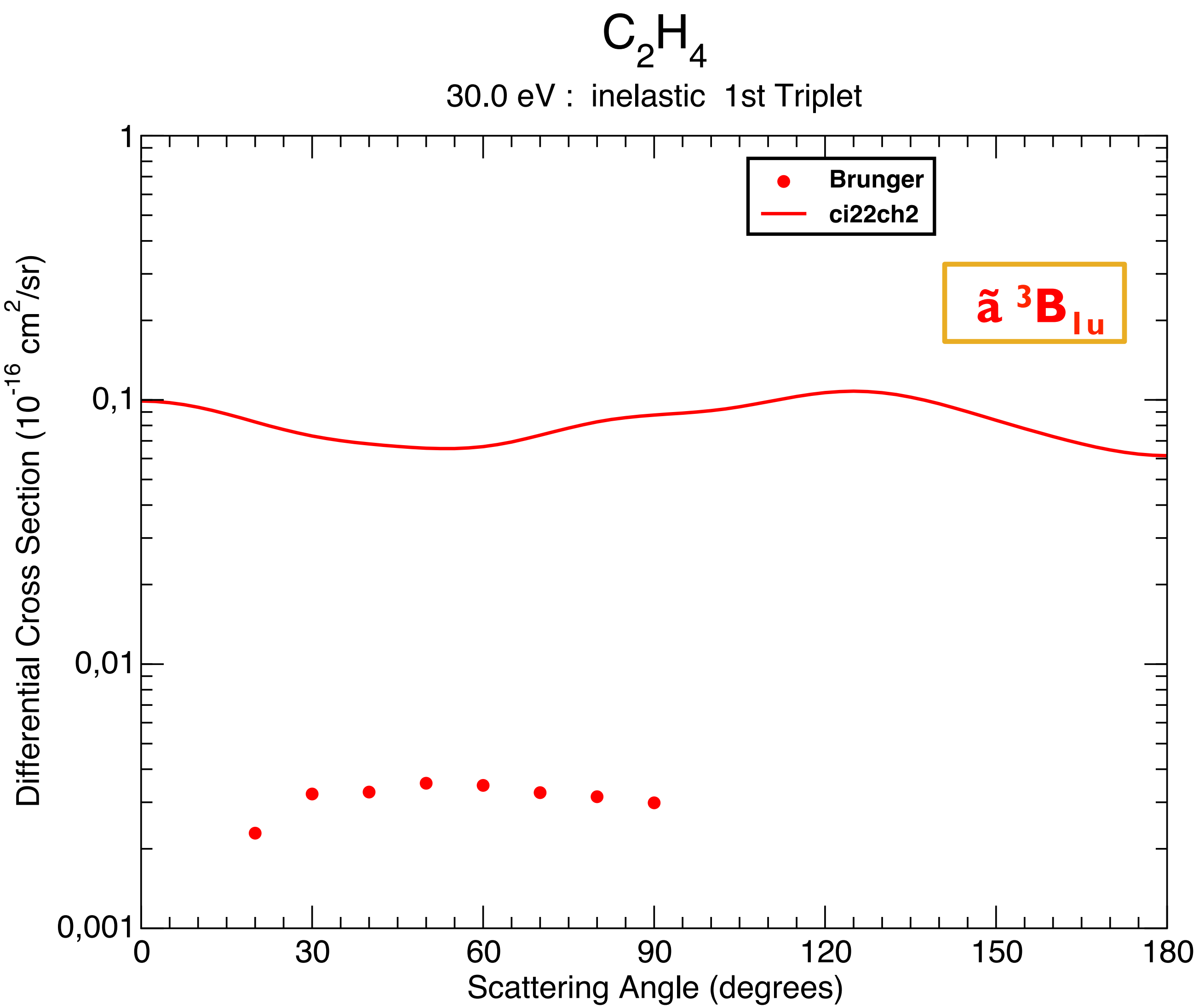
Bullets are Michael Allan's experiments.

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

APS physics

R. F. da Costa, M. H. F. Bettega, M. T. do N. Varella, E. M. de Oliveira and M. A. P. Lima, *Phys. Rev.A* **90**, 052707 (2014).

Surprisingly, at higher energies the agreement is not good!!



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R. F. da Costa, M. H. F. Bettega, M. T. do N. Varella, E. M. de Oliveira and M. A. P. Lima, *Phys. Rev. A* **90**, 052707 (2014).

Only 22 pairs
Hole-particle

TABLE I. Calculated and experimental excitation energies for ethylene. Up to 20, 30 and 50 eV, the FSCI spectrum is composed by 138, 260 and 402 electronically excited states, respectively. The MOBSCI calculations at these energies were performed with 45 excited states, where 17 of them are physical excited singlets or triplets states and the others are pseudostates.

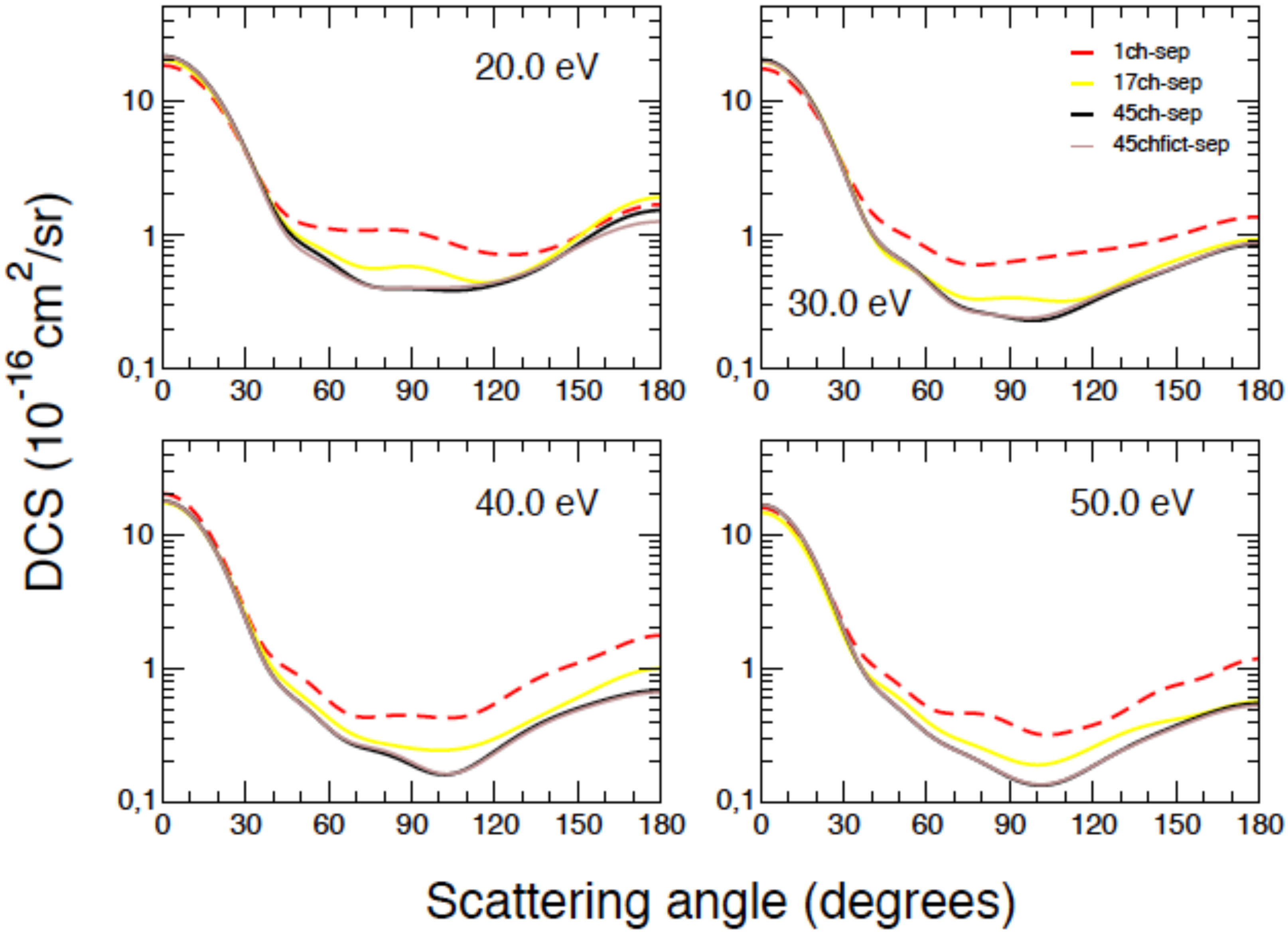
	Energy (eV)		
	FSCI	MOBSCI	Expt.
TRIPLET	3.56	3.60	4.36[a]
	6.90	6.92	6.98[a]
	7.73	7.75	7.79[a]
	8.48	8.83	8.15[b]
	8.80	9.08	8.57[b]
	9.06	9.19	
	9.42	9.58	
	9.48	9.73	
	9.54	9.74	
SINGLET	7.11	7.13	7.11[b]
	7.83	7.85	7.80[b]
	7.88	8.55	7.90[b]
	8.99	9.28	8.28[a]
	9.24	9.37	8.62[b]
	9.25	9.54	8.90[a,b]
	9.63	9.71	9.10[a]
			9.33[a]
			9.51[a,c]
			9.62[a]

[a] Experimental data from Ballard *et al.* [24].

[b] Experimental data from Do *et al.* [16].

[c] For this energy were found two states.

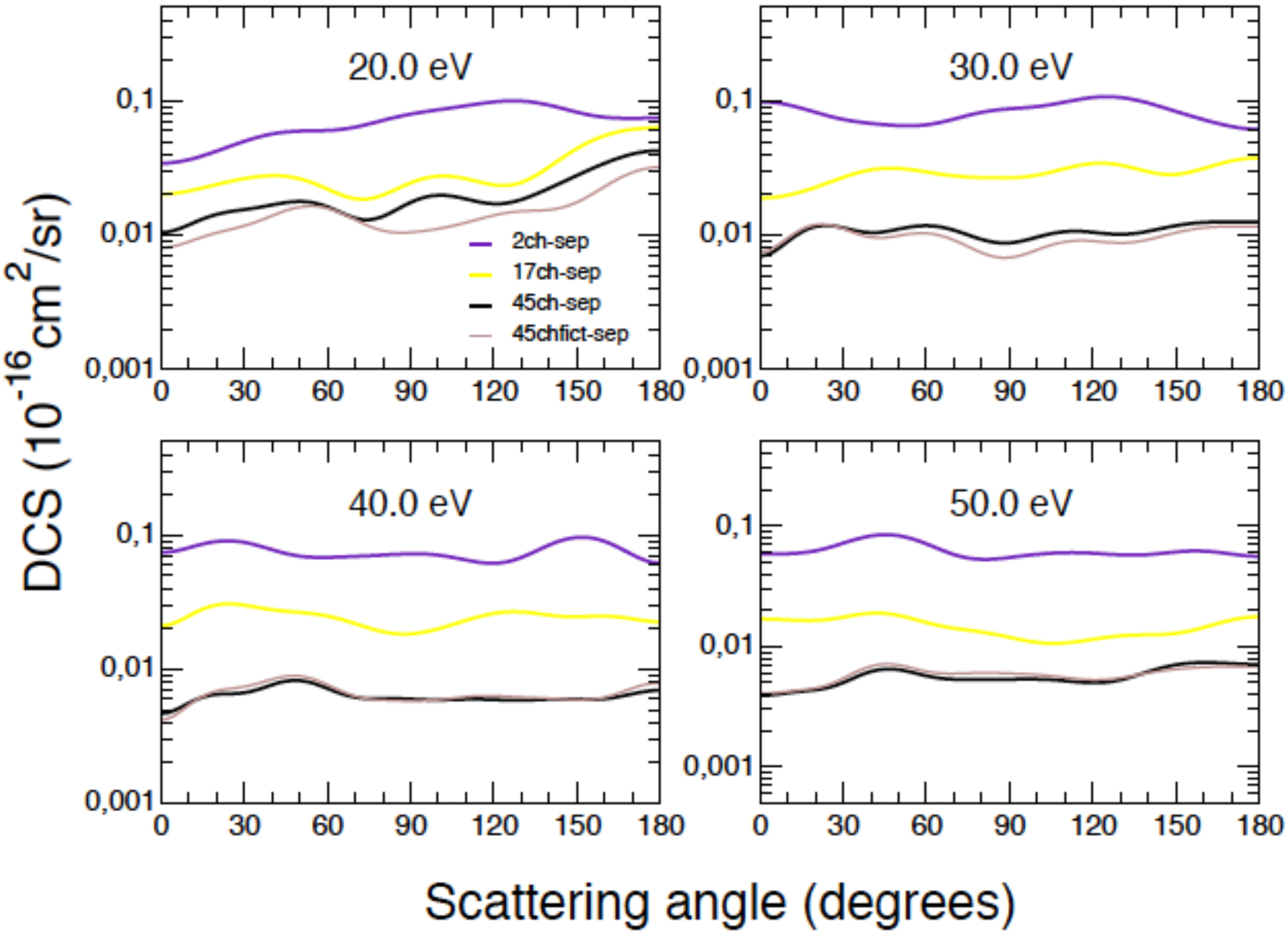
Flux dynamics in the elastic channel for e^{-}-C_2H_4 scattering



R. F. da Costa, M. H. F. Bettega, M. T. do N. Varella, E. M. de Oliveira and M. A. P. Lima, *Phys. Rev. A* **90**, 052707 (2014).

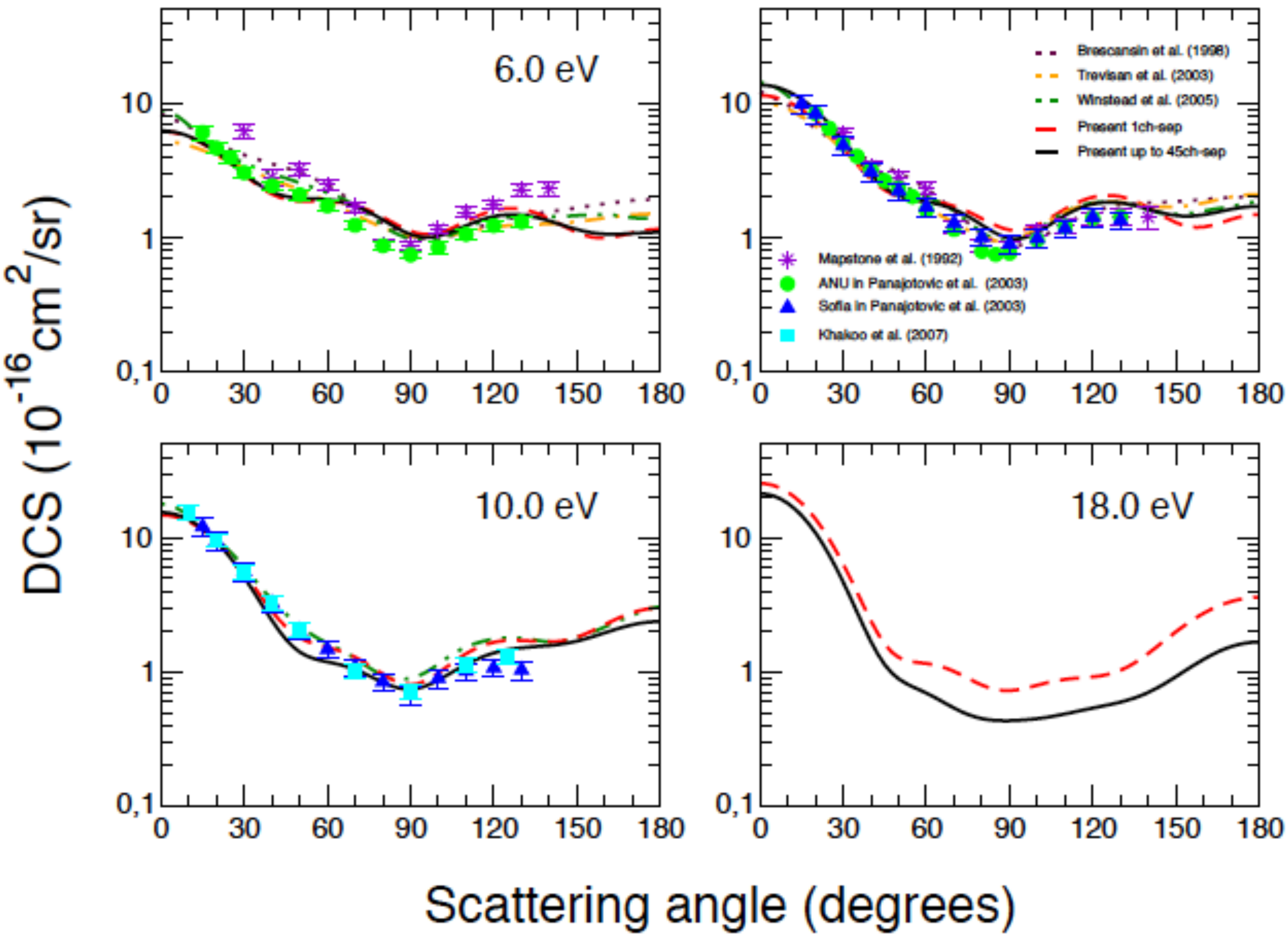
Flux dynamics to the (1st triplet) inelastic channel for e^--C_2H_4 scattering

$\tilde{a}\ ^3B_{1u}$



R. F. da Costa, M. H. F. Bettega, M. T. do N. Varella, E. M. de Oliveira and M. A. P. Lima, *Phys. Rev. A* **90**, 052707 (2014).

Elastic channel for lower energies in e^--C_2H_4 scattering



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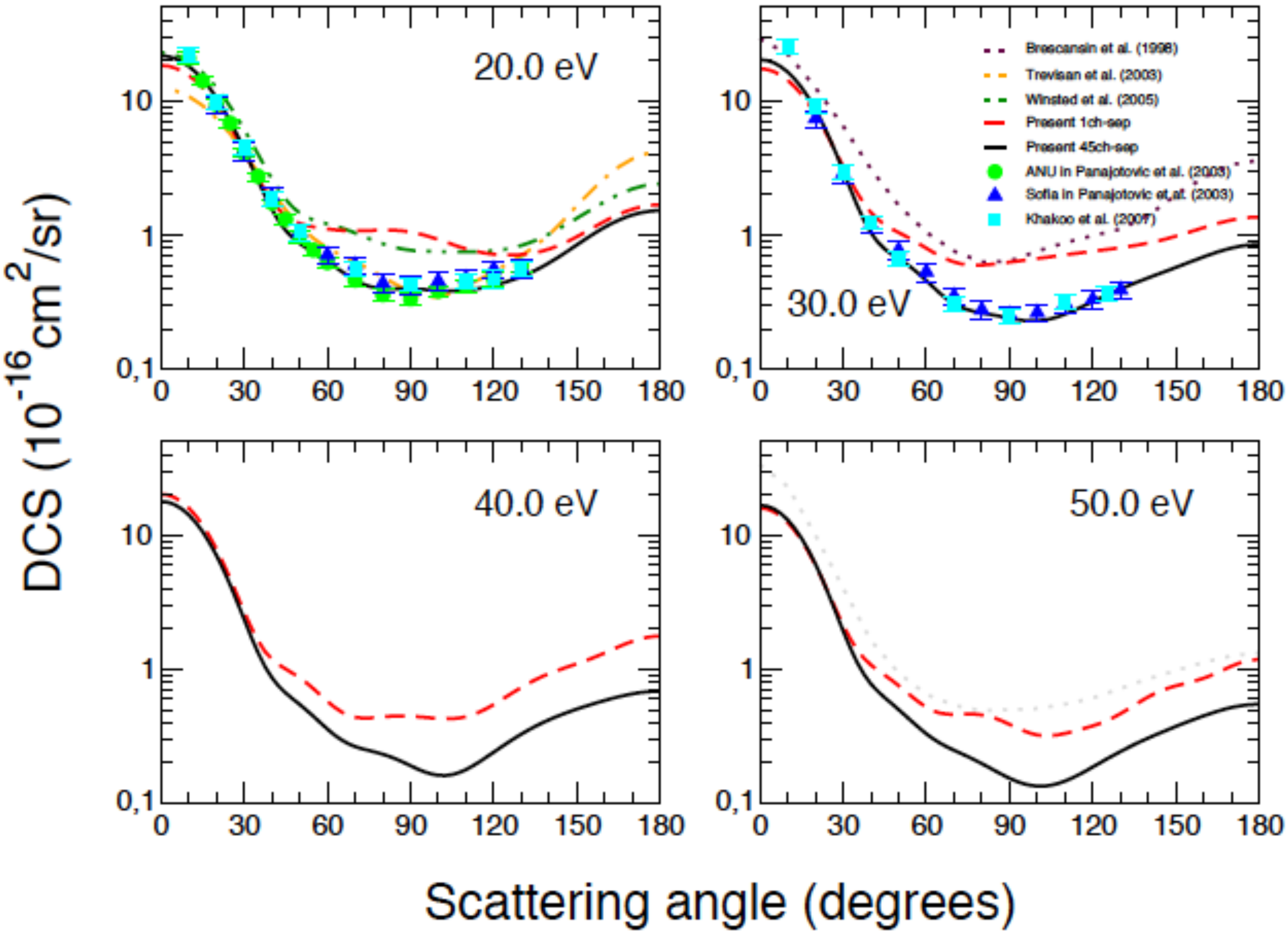
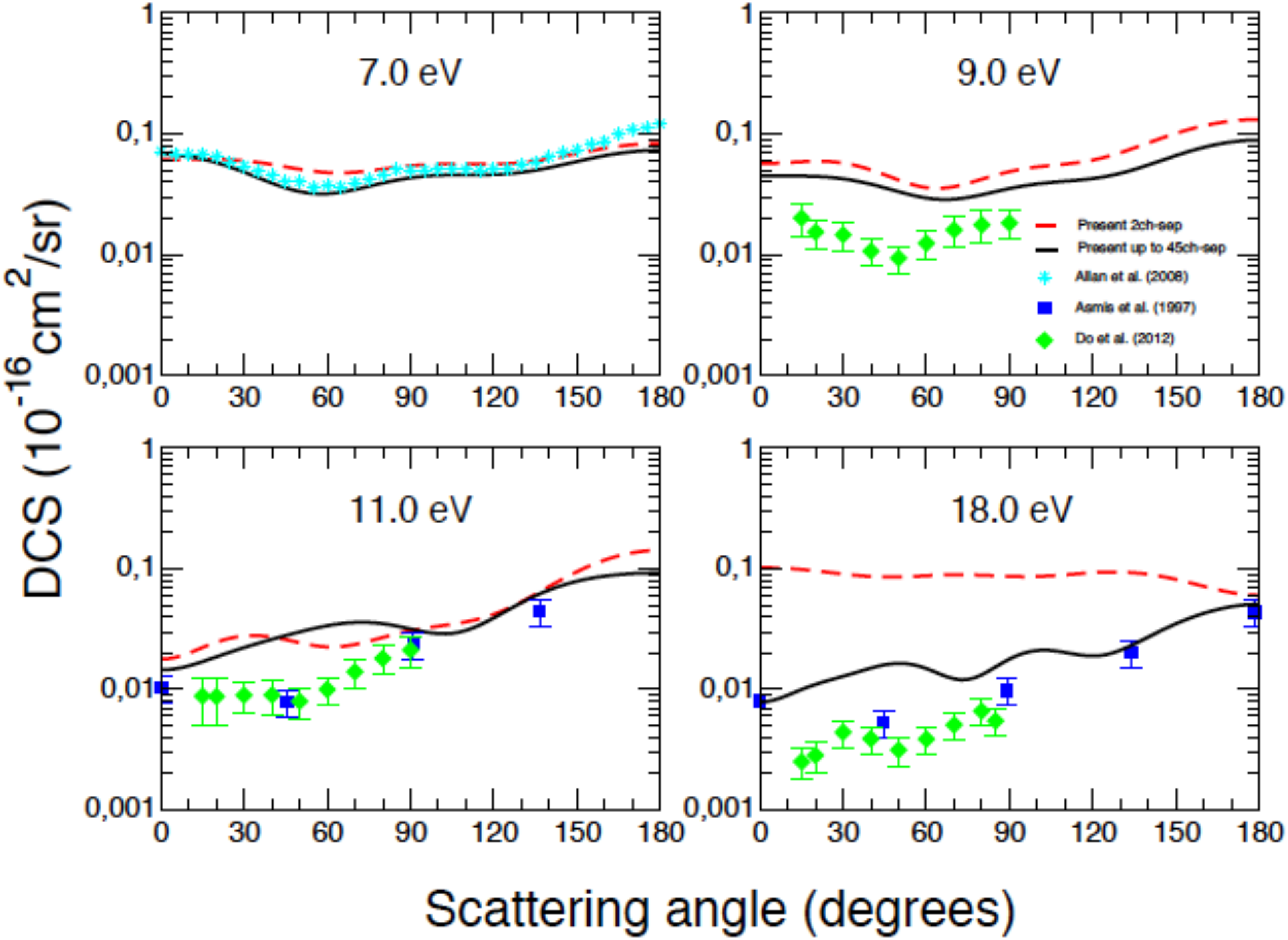
Elastic channel for higher energies in e^{-}-C_2H_4 scattering



R. F. da Costa, M. H. F. Bettega, M. T. do N. Varella, E. M. de Oliveira and M. A. P. Lima, *Phys. Rev. A* **90**, 052707 (2014).

Inelastic channel (1st triplet) for lower energies in e^--C_2H_4 scattering

ã $^3B_{1u}$



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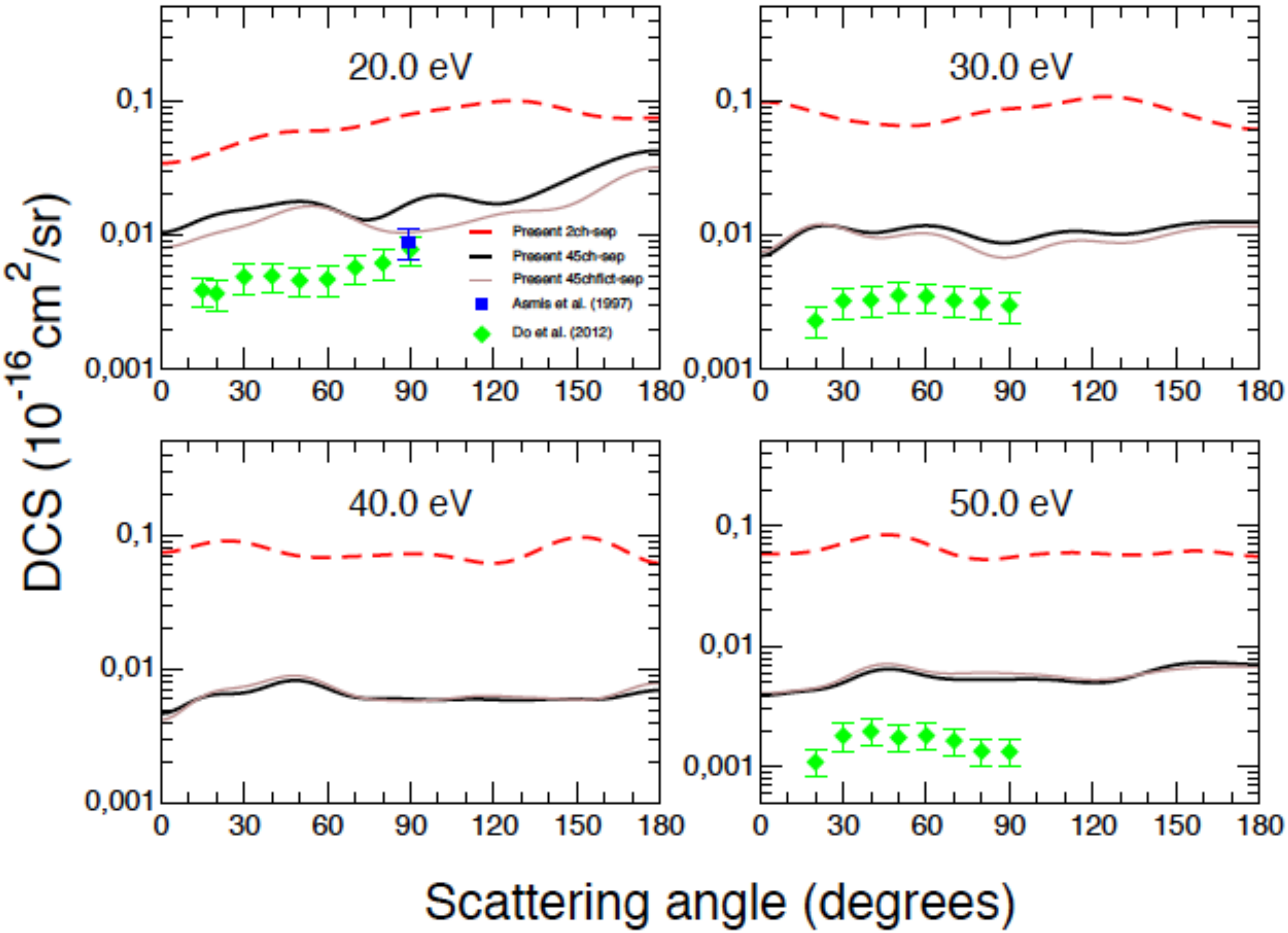
Inelastic channel (1st triplet) for higher energies in e^--C_2H_4 scattering

ã $^3B_{1u}$



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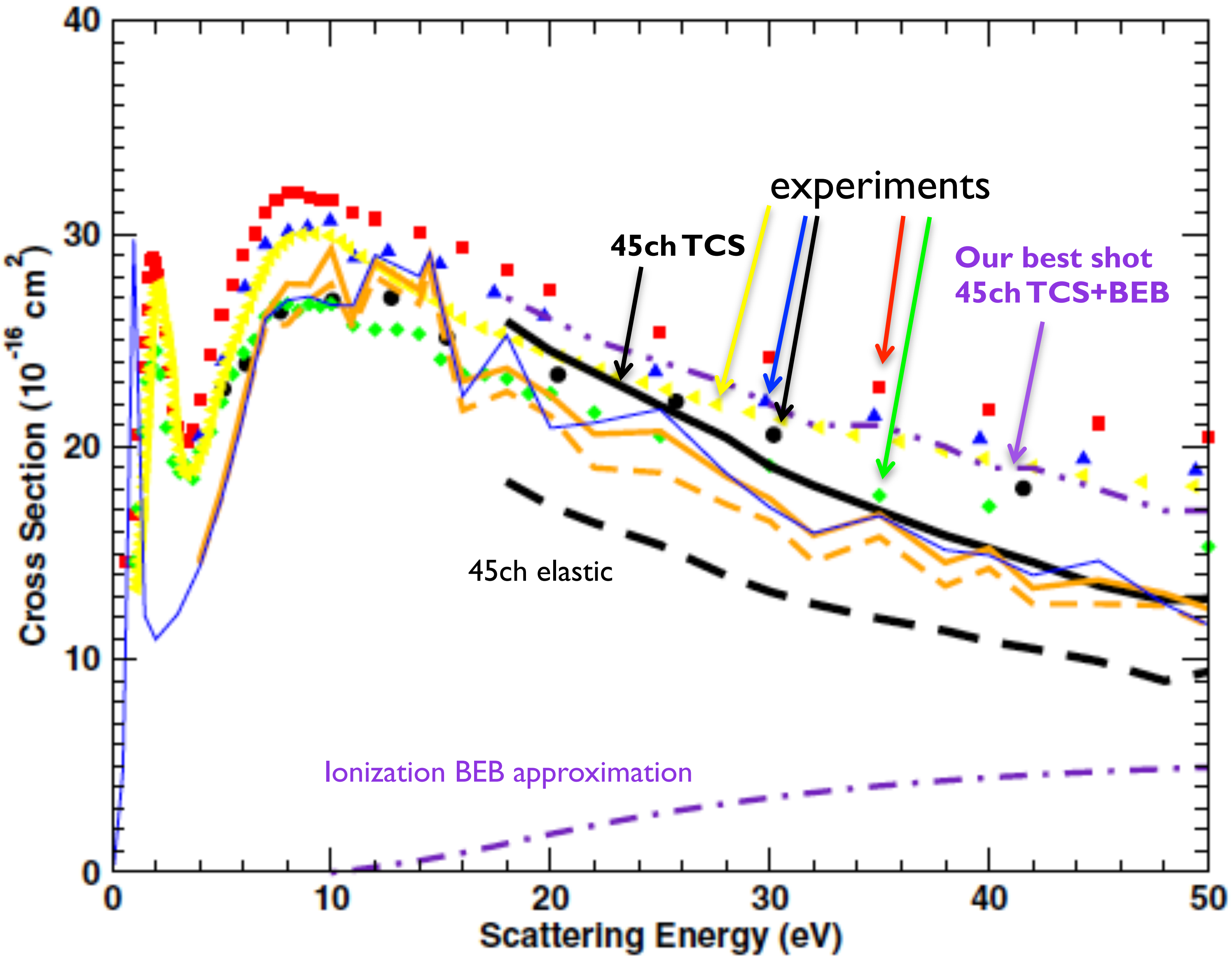
Total cross section for e^--C_2H_4 scattering



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