Electronic excitation of molecules by electron impact with the Schwinger Multichannel Method with Pseudopotentials (SMCPP): how far has it gone?

by

Marco A. P. Lima
Unicamp

REVIEWING MOTIVATIONS

Electron scattering by Molecules

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

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

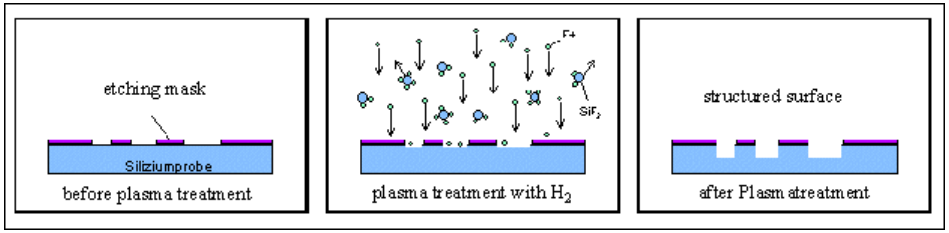
and got further motivated by great applications

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

Surface treatment with Plasmas

Plasma Processing Gases → Several Industry Applications

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



IMPROVEMENT NEEDS MODELING AND MODELING NEEDS DATA

Modeling is a big challenge

Electron collision data: cross sections for

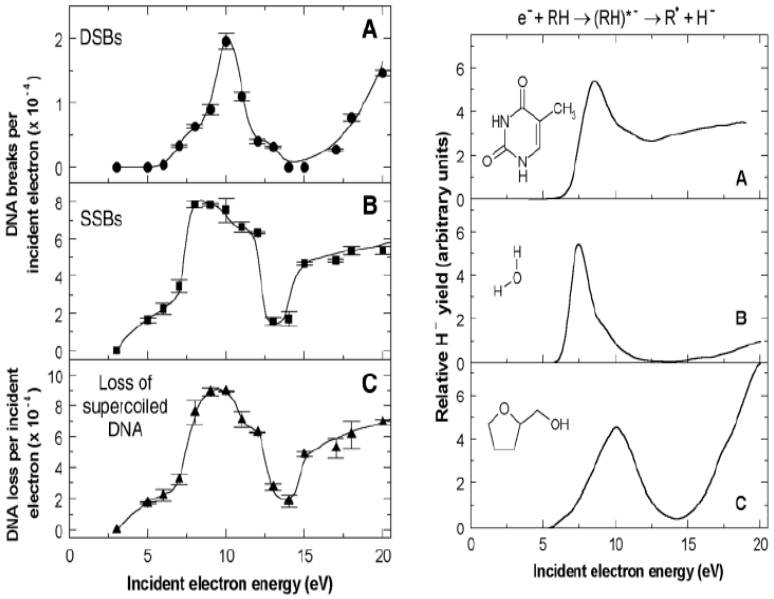
Elastic
Inelastic: electronic, rotational and vibrational excitation
Ionization
Dissociation

Electron-Induced Damage to Biomolecules

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

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



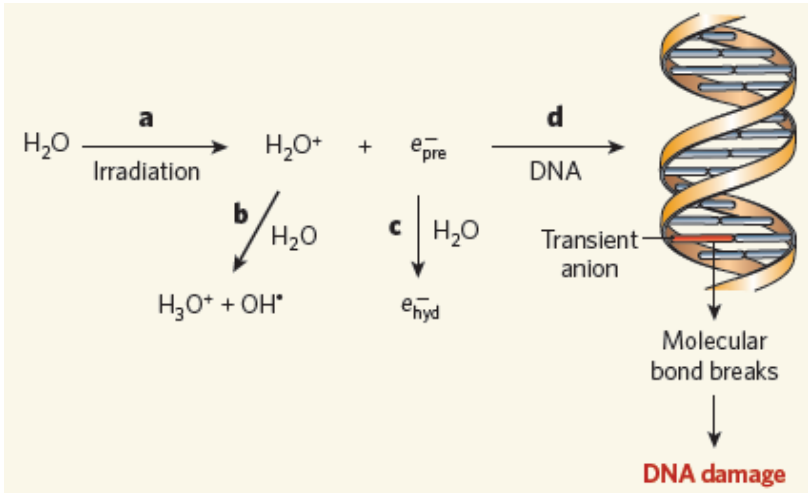
Science, **287** 1658 (2000)

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)

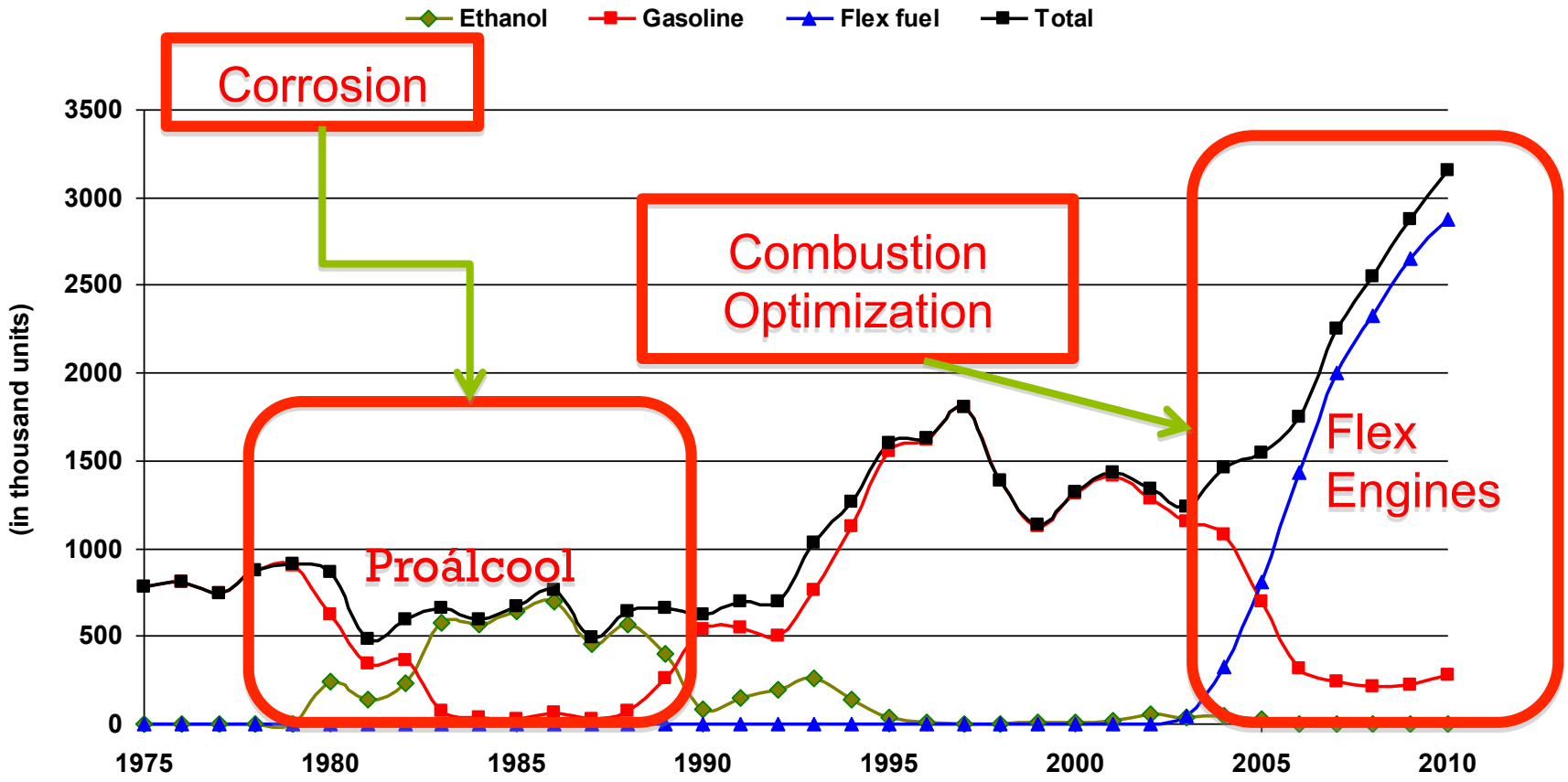
J|A|C|S COMMUNICATIONS

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

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

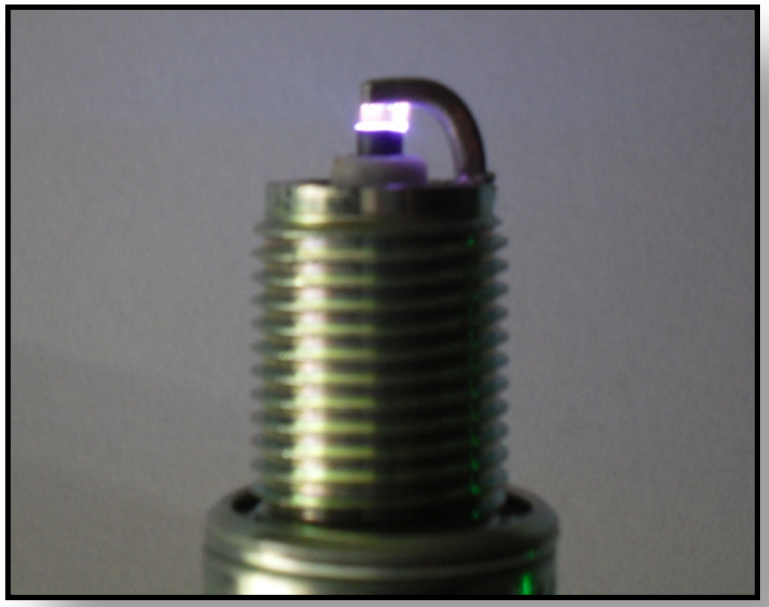
SPECIAL MOTIVATION

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



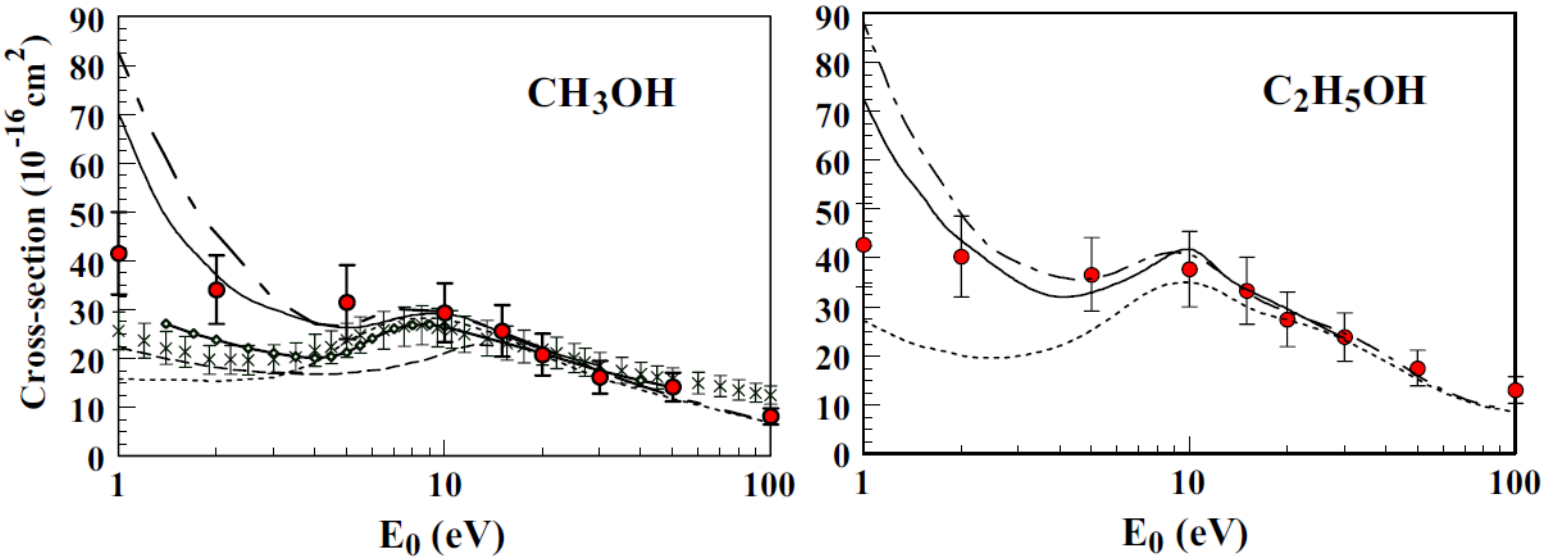
Theoretical support for an application project working on:

- 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

Special motivation II: large scale production of ethanol

Biomass: a source of energy and carbon

Special motivation II: large scale production of ethanol

Biomass: a source of energy and carbon

Special motivation II: large scale production of ethanol

First generation ethanol: crushing the cane for the juice

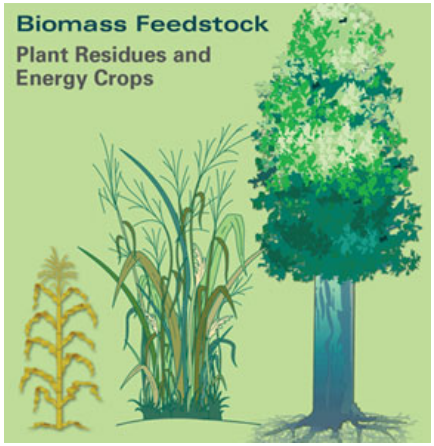
Special motivation II: large scale production of ethanol

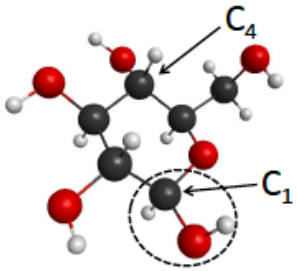
Bagasse piles at the mill.

2nd generation ethanol?
Other high value bioproducts?

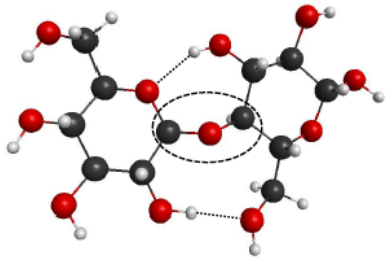
Can we use plasmas on Biomass?

Biomass is Made Up with Fermentable Sugars

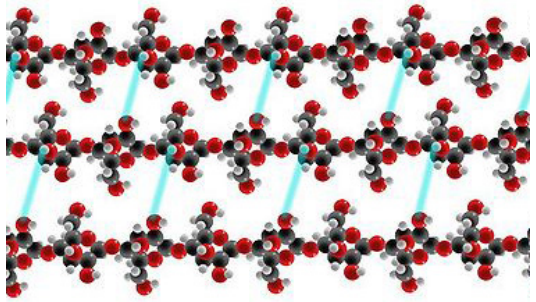


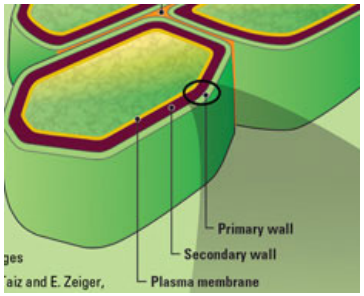


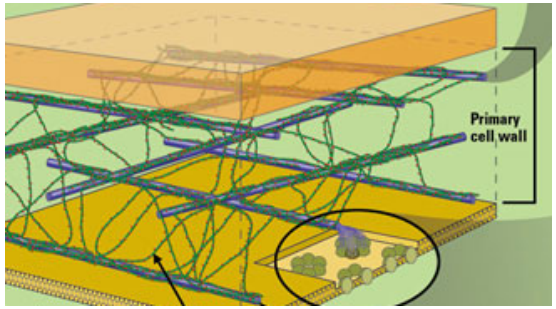
β-D-glucose

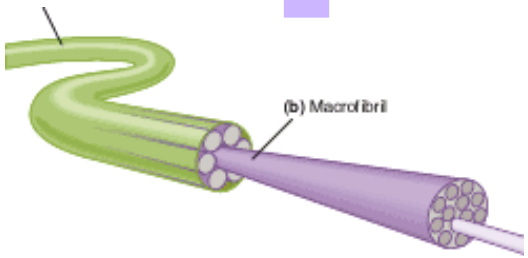


cellobiose

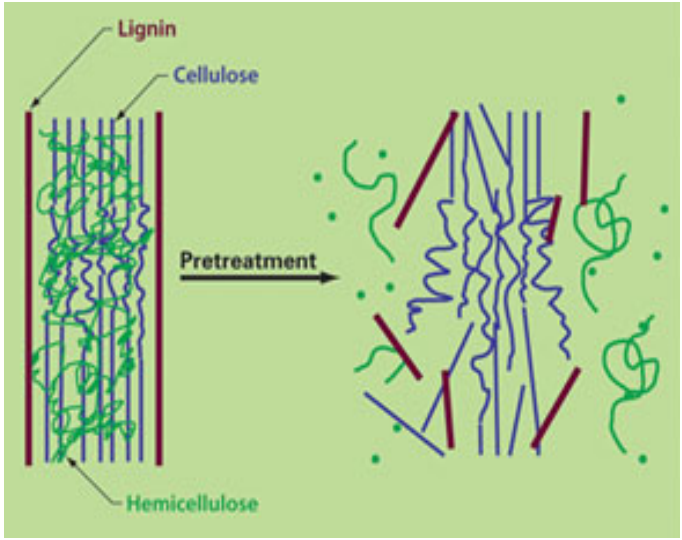




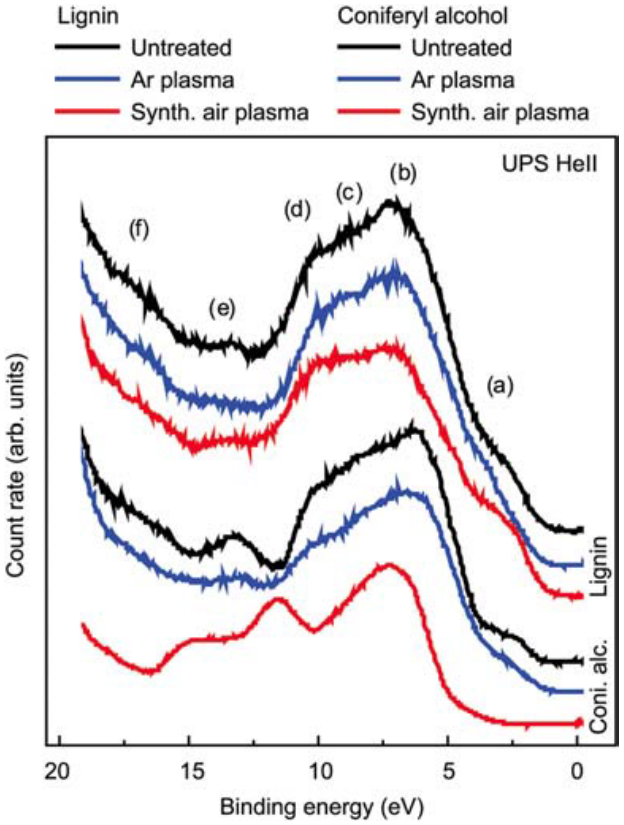


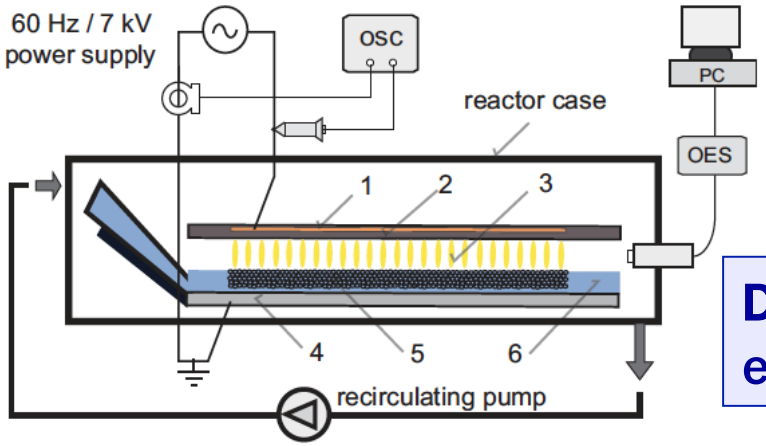


Lignocellulose is Resistant to Hydrolysis



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





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

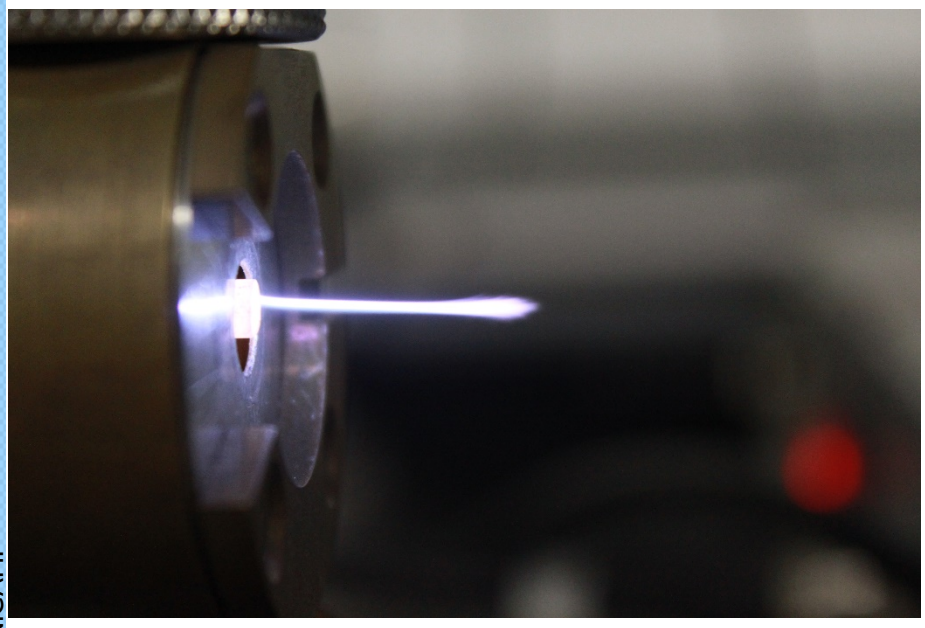
Holzforschung, Vol. 64, pp. 331–336, 2010

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

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

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.

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

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

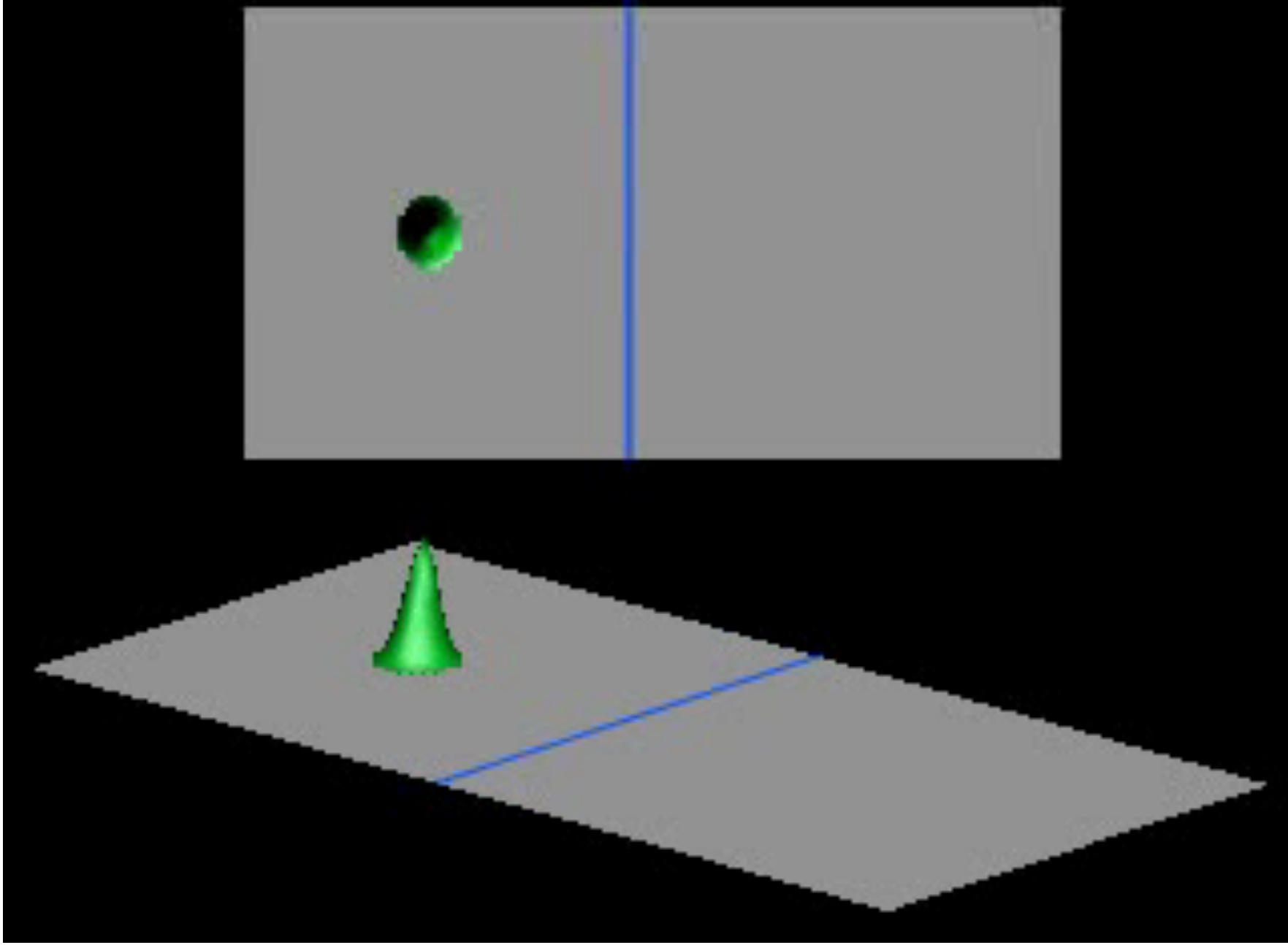
Asymptotic condition

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

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

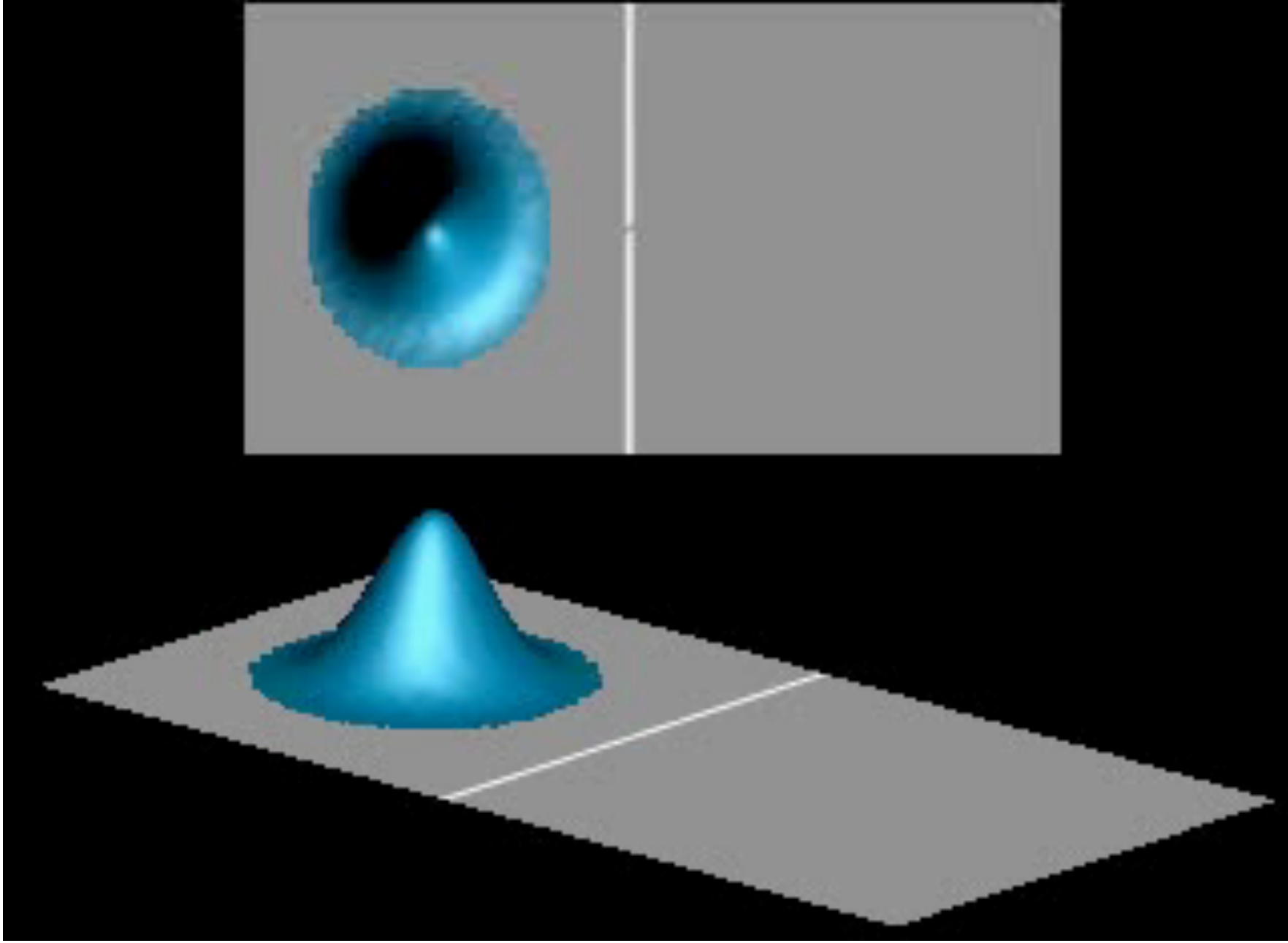
Differential cross section

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



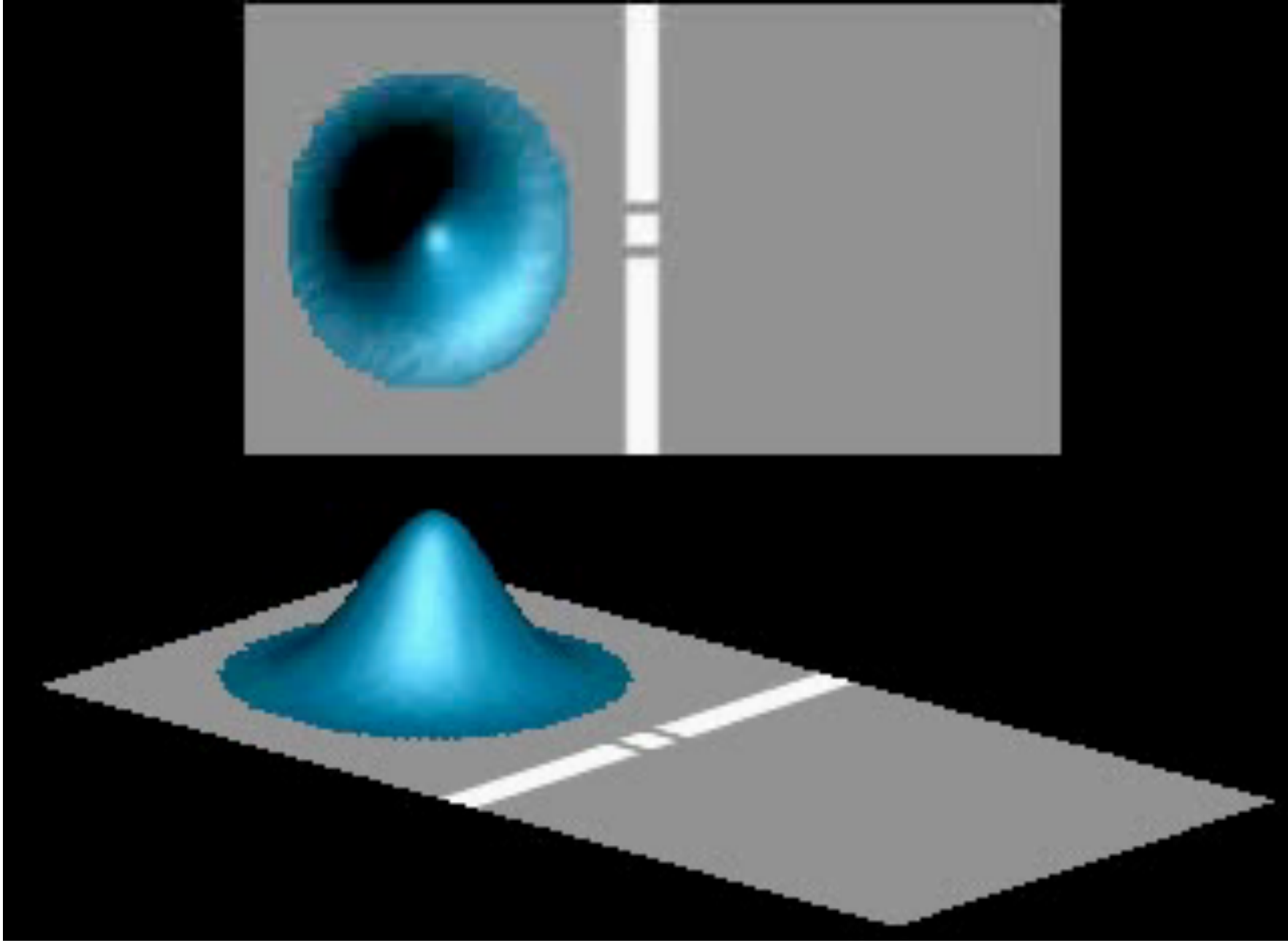
Tunnel effects: access to classical forbiden regions

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



diffraction: like in one slit experiments

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



interference – like in two slit experiments

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

Scattering theory

Schrödinger differential equation

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

Within the Fixed-nuclei approximation

Lippmann-Schwinger integral equation

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

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

Target is a many-body problem

Free-particle Green's function

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

Numerical integration

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

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

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

$A^{(\pm)}|\Psi_{\mathbf{k}}^{(\pm)}\rangle = V|S_{\mathbf{k}}\rangle$ *is equivalent to* $H|\Psi_{\mathbf{k}}^{(\pm)}\rangle = E|\Psi_{\mathbf{k}}^{(\pm)}\rangle$ *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 $P \equiv \sum_{\ell=1}^{open} |\Phi_\ell\rangle\langle\Phi_\ell|$ 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):

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

Truncation must take place

Cartesian Gaussian expansion

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)

Coupling level

- Elastic scattering with and without polarization effects

1. 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

2. 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

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

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 (MOBSCI Minimum Orbital Basis for Single-excitation Configuration Interaction, Ph.D. Thesis of da Costa)

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

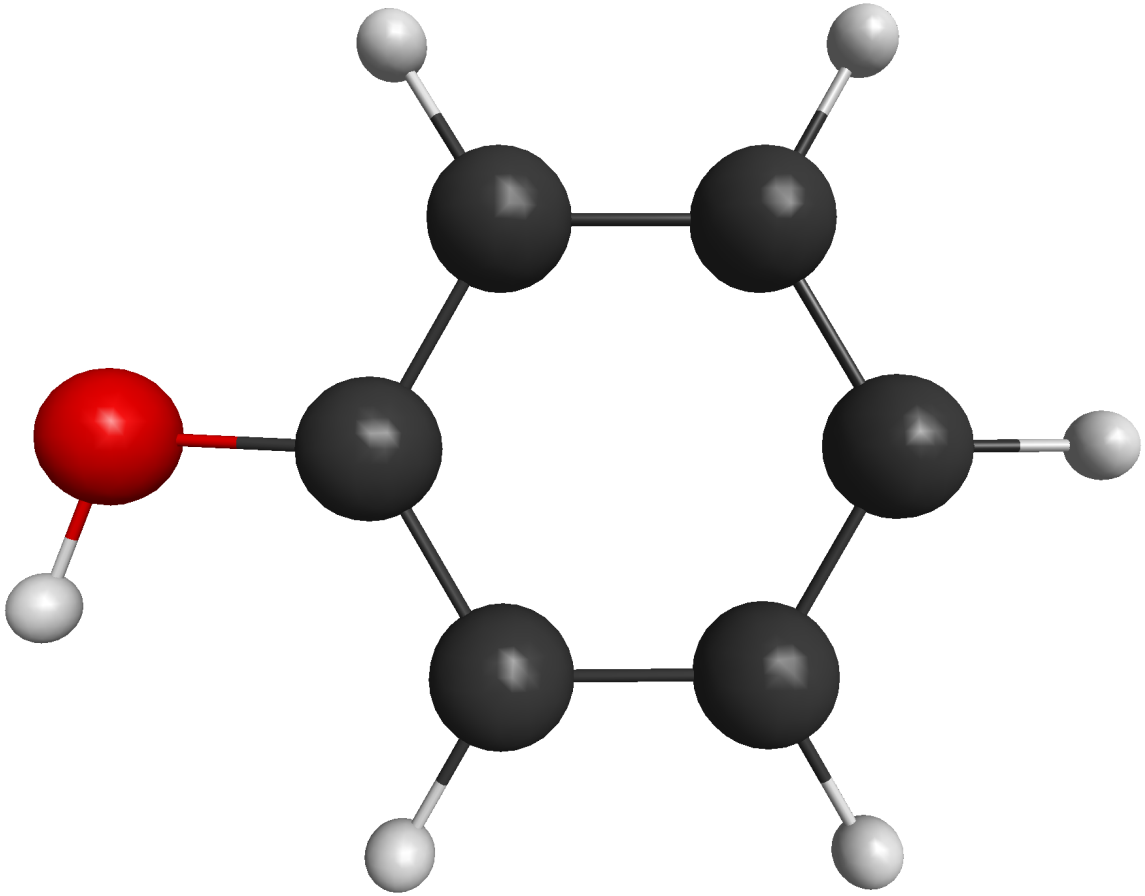
All this with pseudopotentials: M. H. F. Bettega, L. G. Ferreira, and M. A. P. Lima, "Transferability of Local-Density Norm-Conserving Pseudopotentials to Electron-Molecule Collision Calculations," *Phys. Rev. A* **47**, 1111-8 (1993)

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

ELECTRONIC EXCITATION

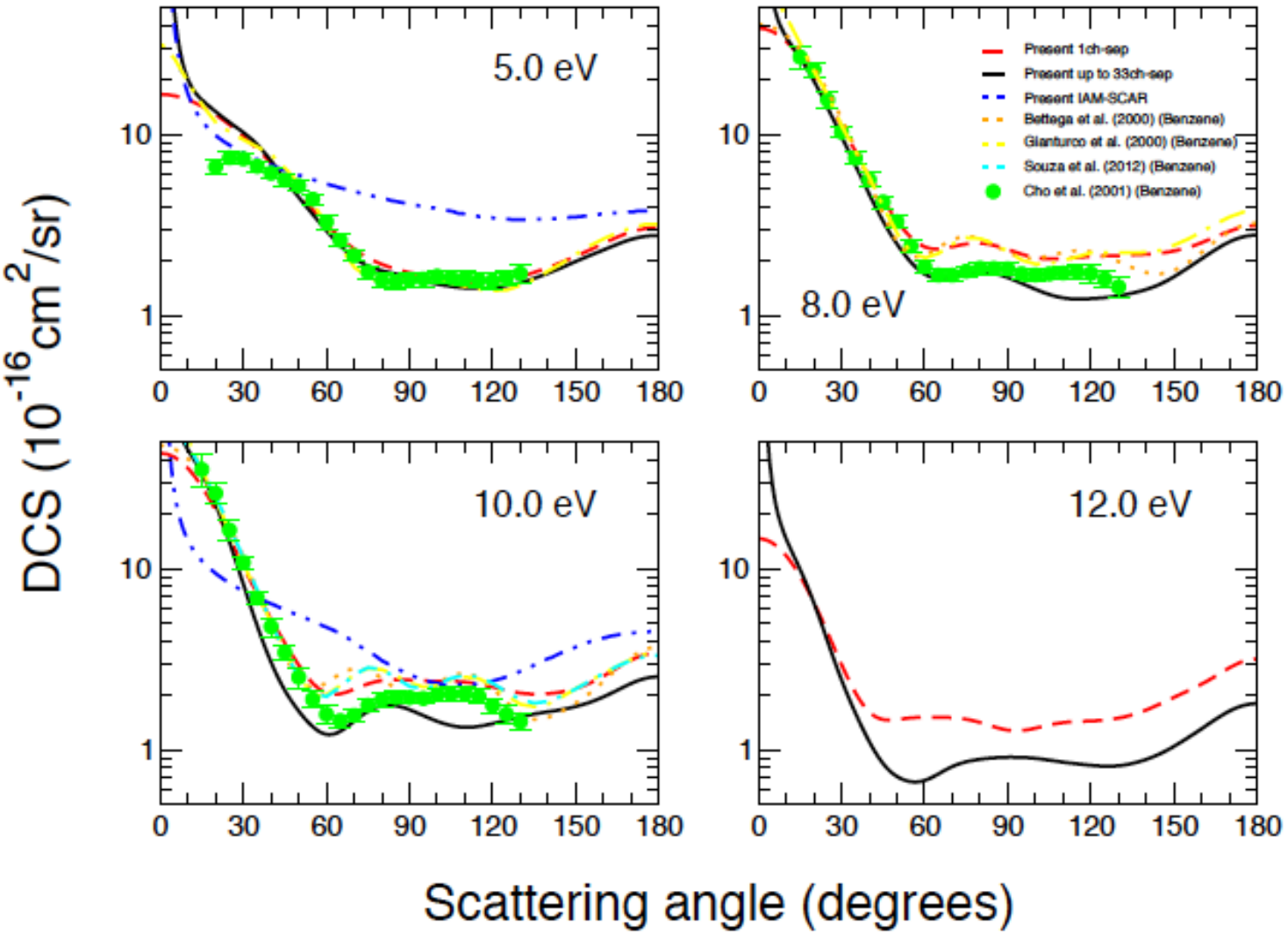
Electronic excitation of Phenol by electron impact

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).



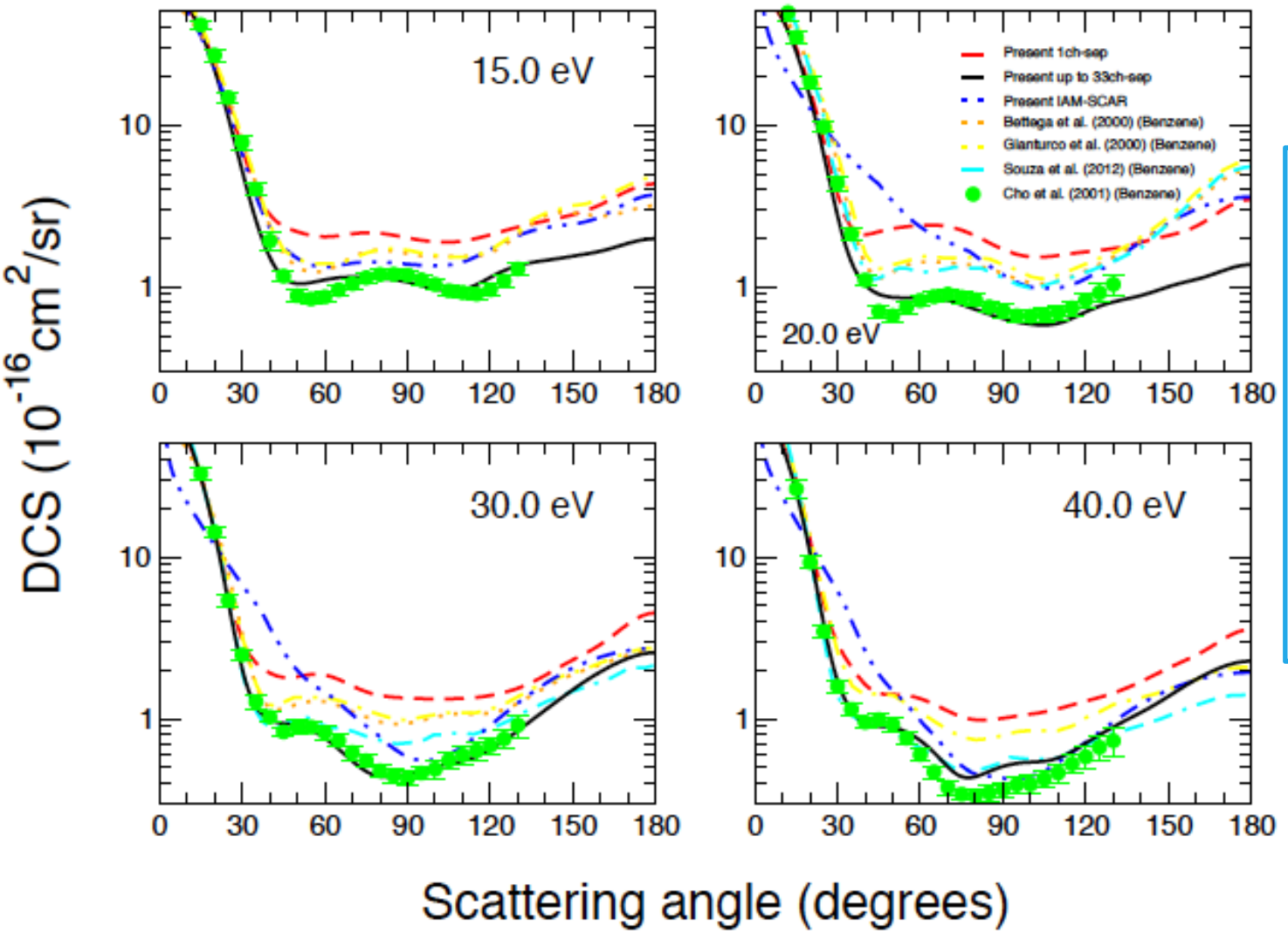
The calculations for the following systems were carried out with the parallel version of the SMCPP code developed by Varella and collaborators

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. Garcia, and M. A. P. Lima, *J. Chem. Phys.* **142**, 104304 (2015).

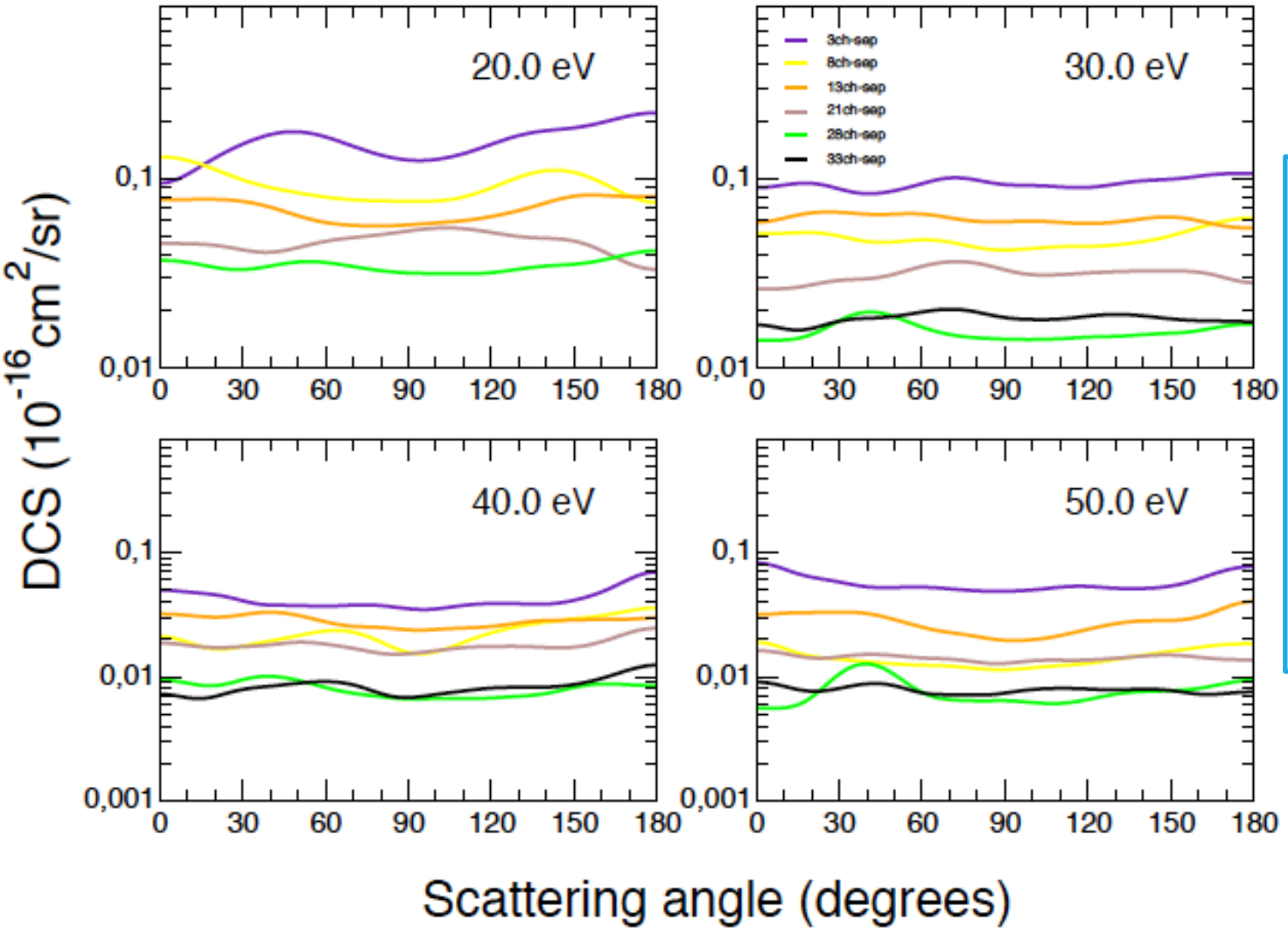
Multichannel coupling on electron-Phenol scattering: Effects on the Elastic channel



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.

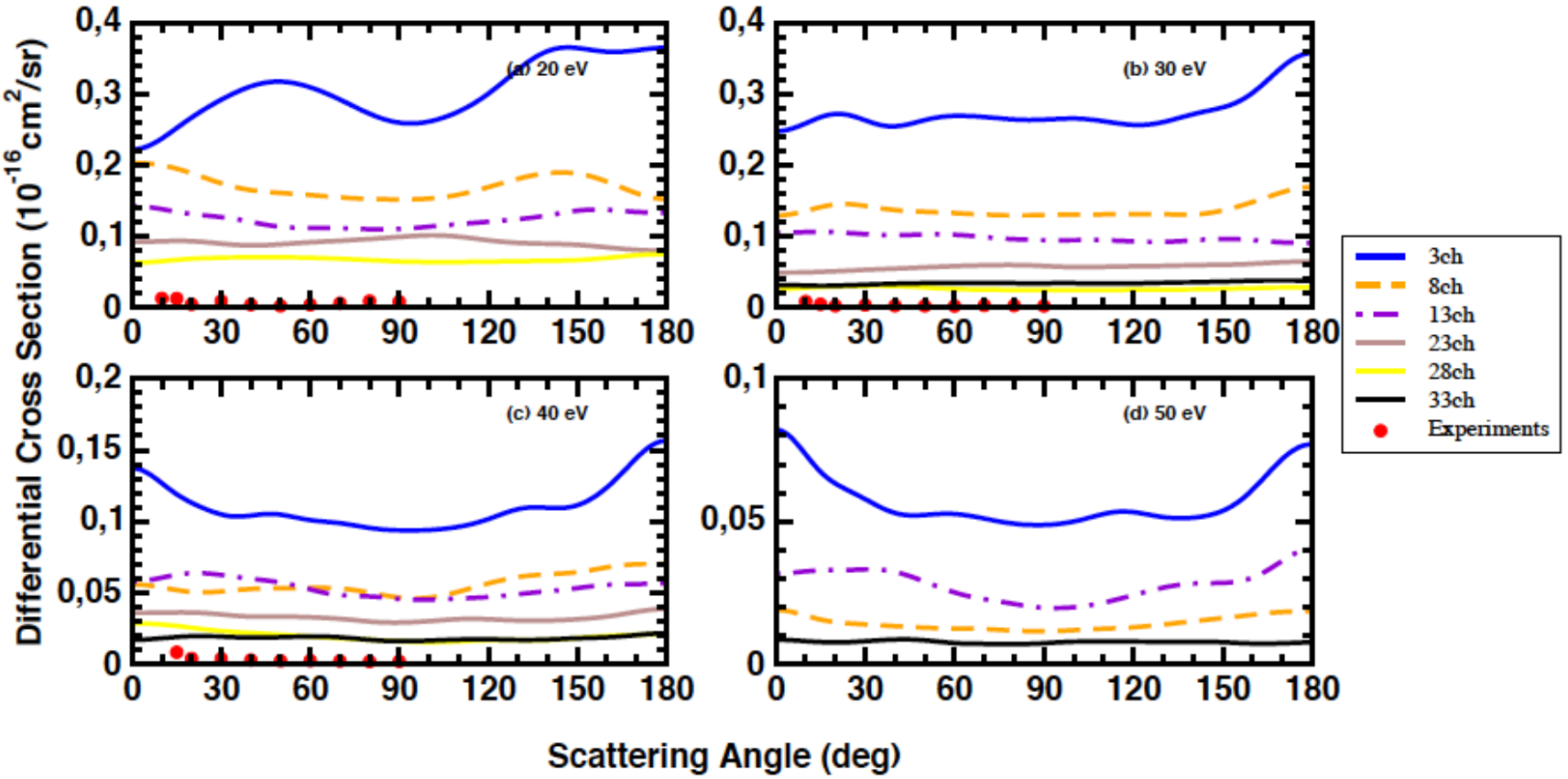
It reminds a classical picture of a river blocked by gates. As you open more gates the flux through all of them decreases.

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. Garcia, and M. A. P. Lima, *J. Chem. Phys.* **142**, 104304 (2015).

Flux competion is also present in the inelastic process

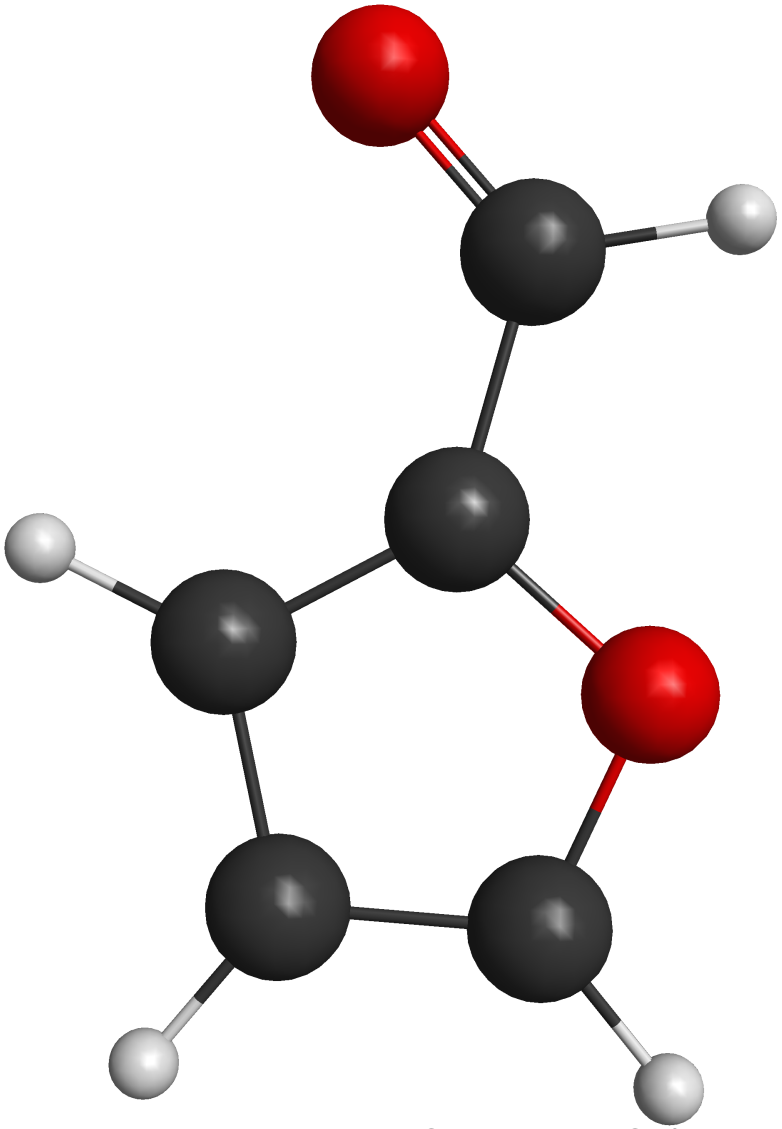
R. F. C. Neves, D. B. Jones, M. C. A. Lopes, K. L. Nixon, G. B. Da Silva, H.V. Duque, E. M. de Oliveira, R. F. da Costa, M.T. do N.Varella, M. H. F. Bettega, M.A. P. Lima, K. Ratnavelu, G. García, and M. J. Brunger, *J. Chem. Phys.* **142**, 104305 (2015).

Phenol: electronic excitation of Band I



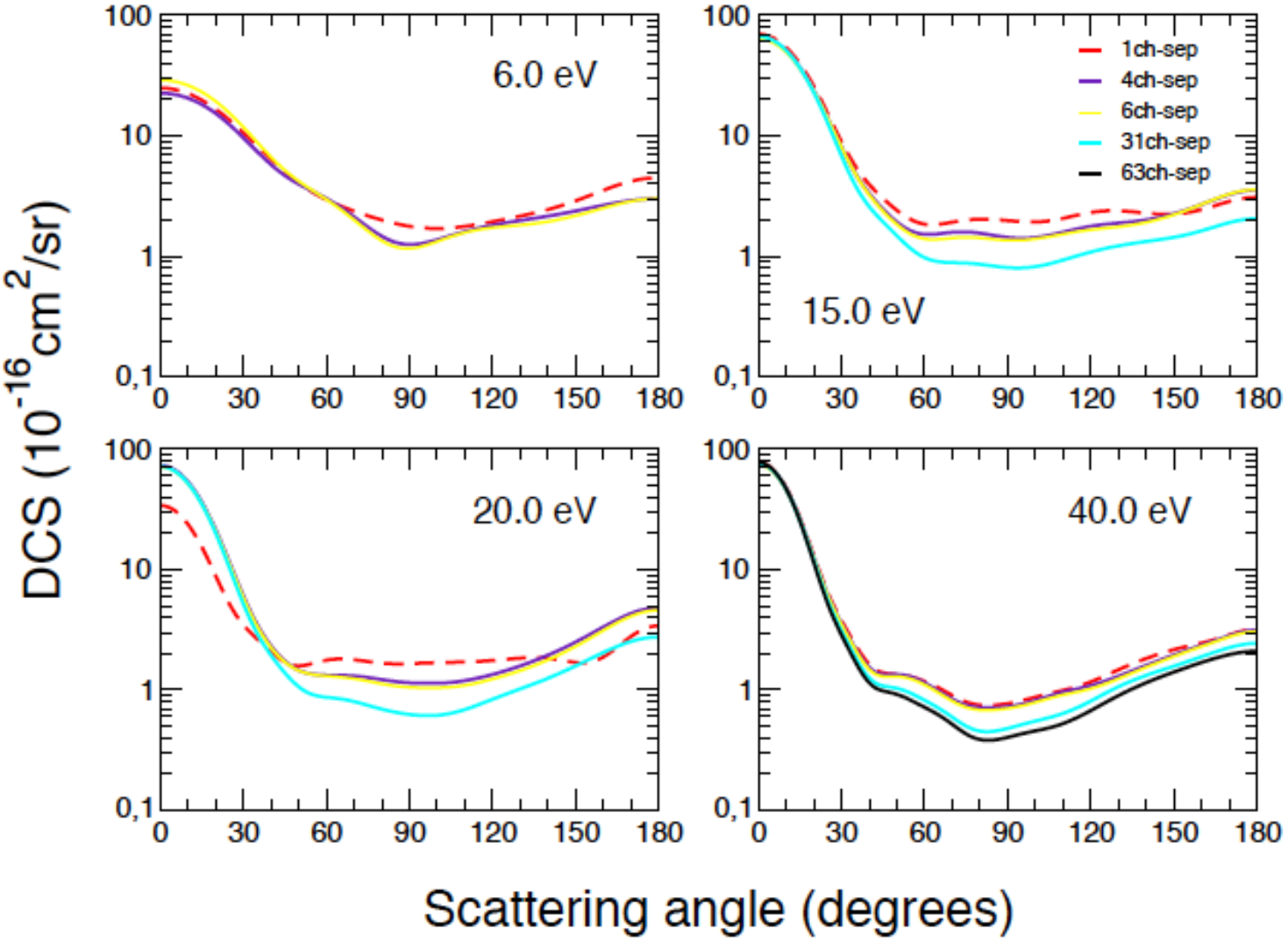
Still a factor of 3-4 from experiments. How would that affect modeling?

Electronic excitation of furfural by electron impact

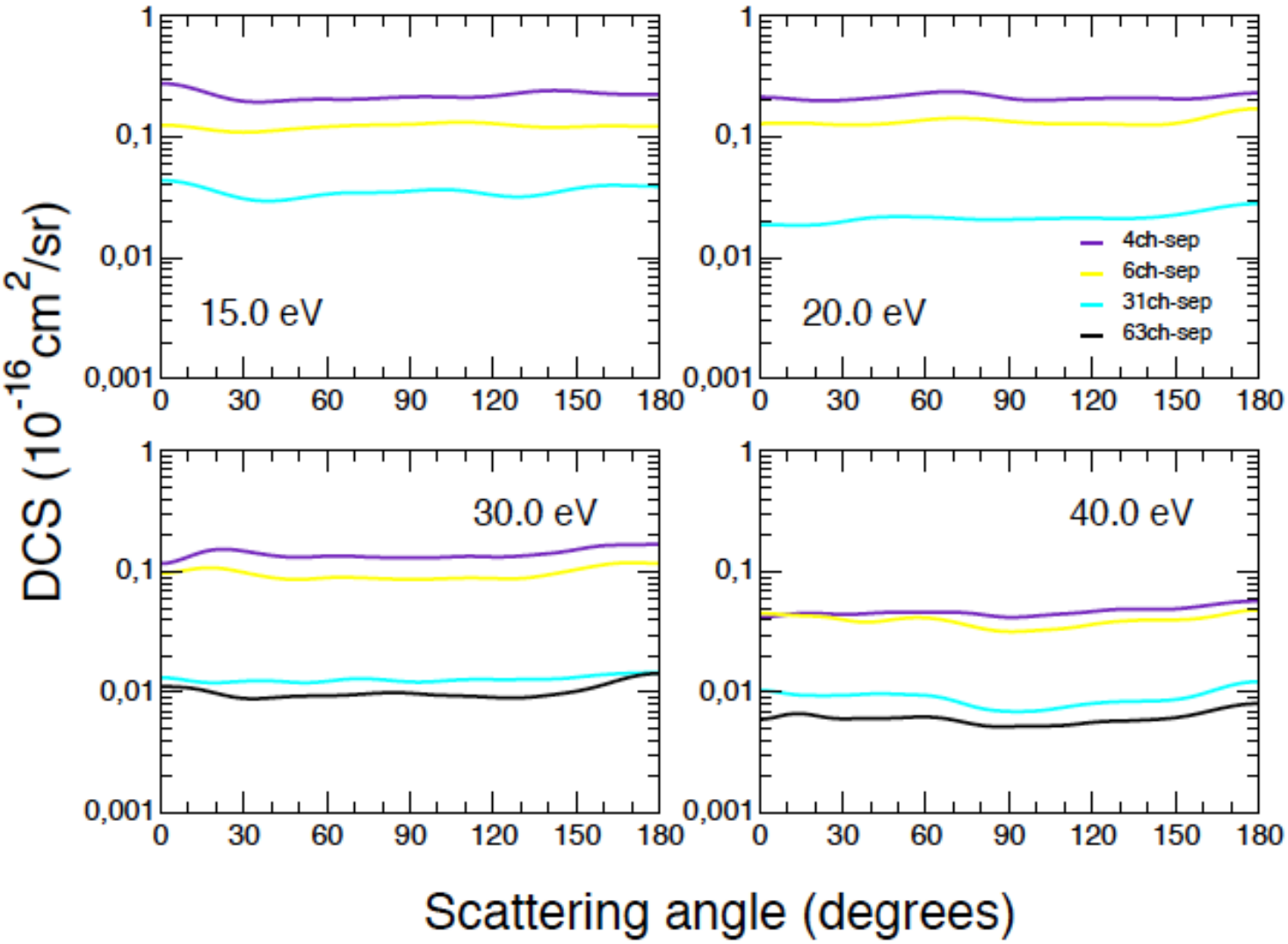


R. F. da Costa, M. T. do N. Varella, M. H. F. Bettega, R. F. C. Neves, M. C. A. Lopes, F. Blanco, G. García, D. B. Jones, M. J. Brunger, *and* M. A. P. Lima, "The electron-furfural scattering dynamics for 63 energetically open electronic states", J. Chem. Phys. **144**, 124310 (2016);

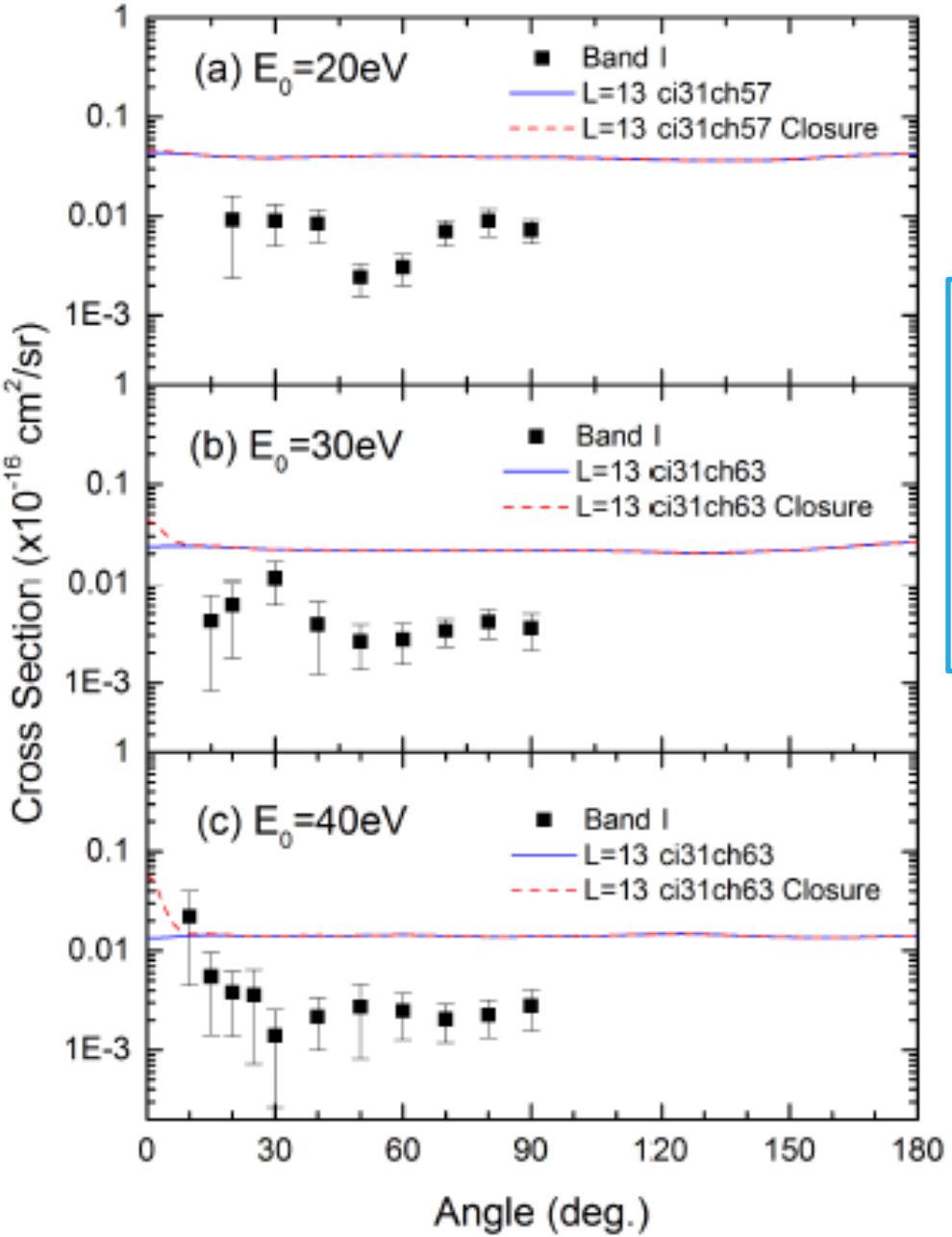
Electronic excitation of furfural by electron impact: Effects on the Elastic channel



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

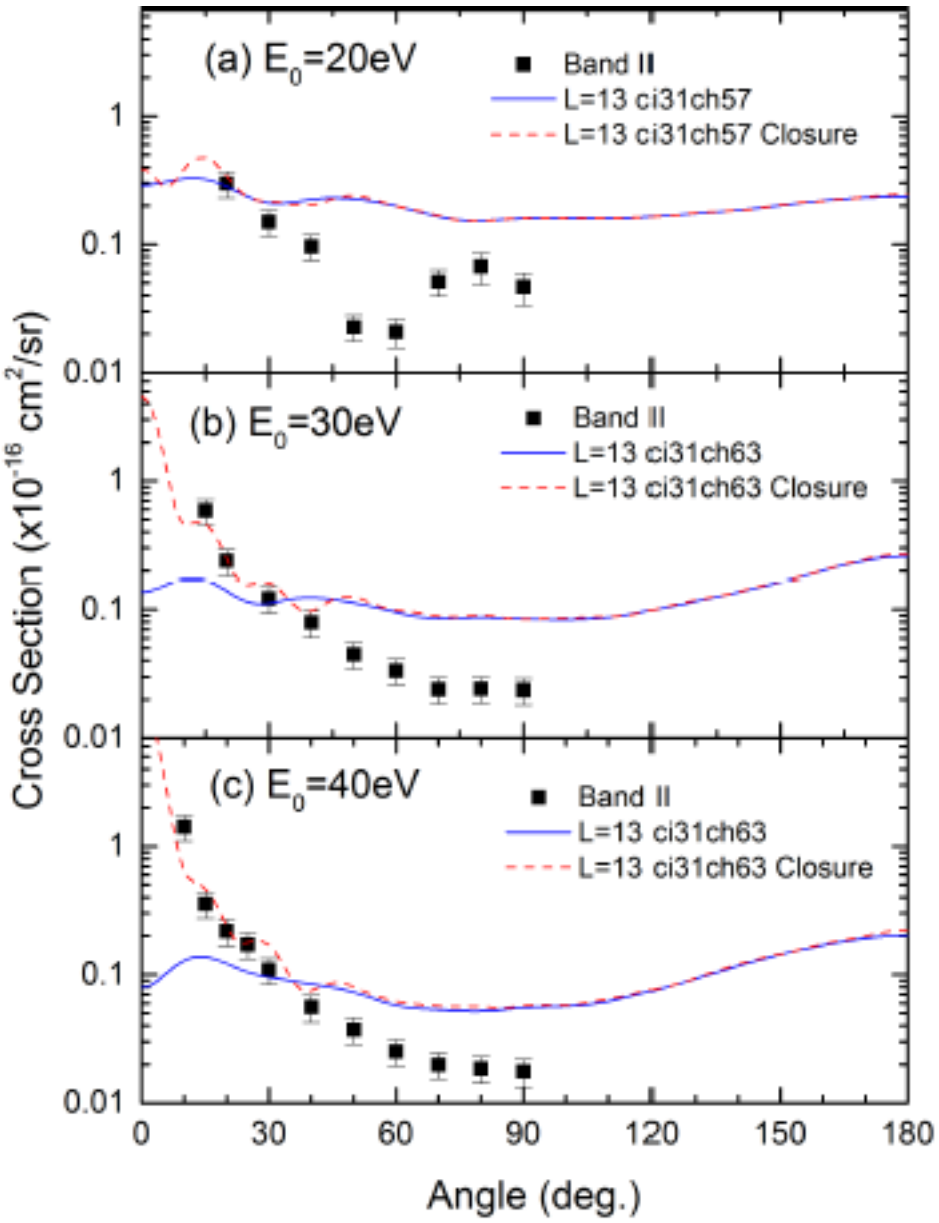


Electronic excitation of Band I of furfural by electron impact:



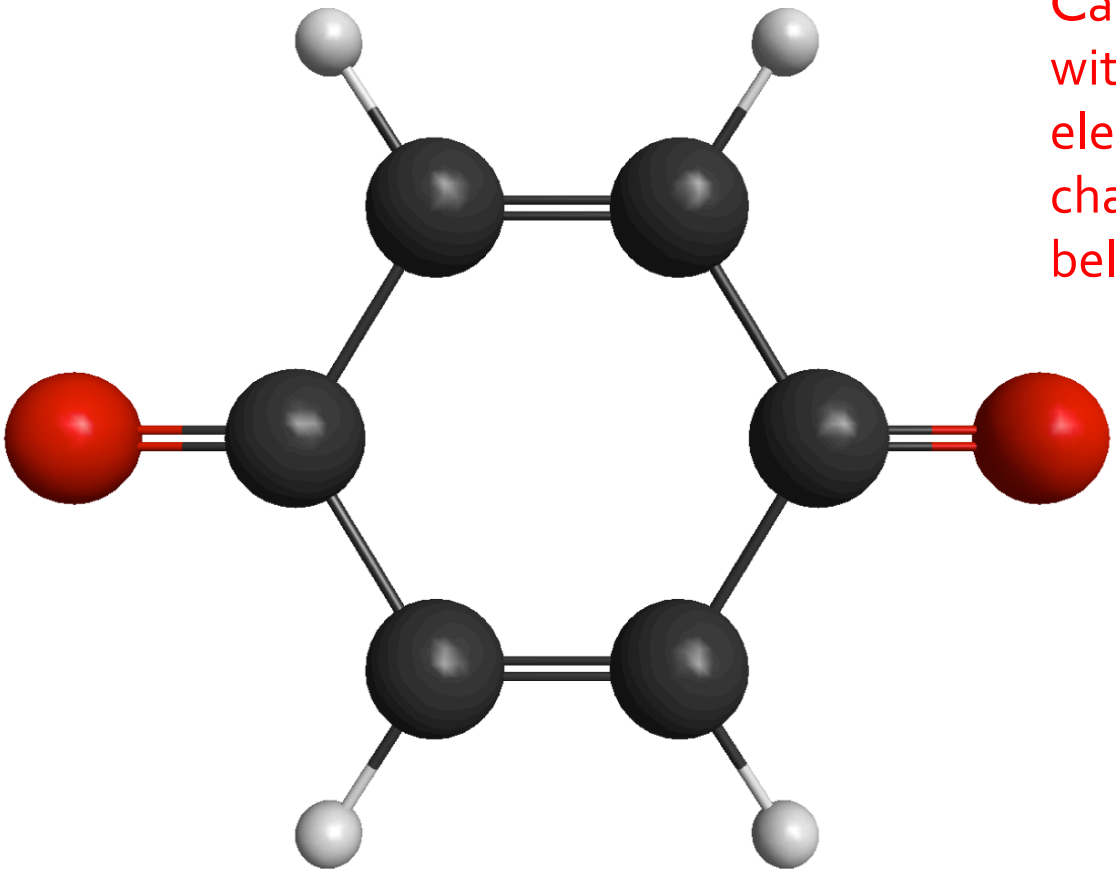
A factor of 3 difference between theory and experiments. Is it good?

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?

Electronic excitation of benzoquinone by electron impact



Calculation with 89 electronic channels below 15,2 eV

R. F. da Costa, J. C. Ruivo, F. Kossoski, M.T. do N.Varella, M. H. F. Bettega, D. B. Jones, M. J. Brunger, *and* M.A. P. Lima, J. Chem. Phys. **149**, 174308 (2018)

New parallel SMCPP computer code developed by Fabris Kossoski

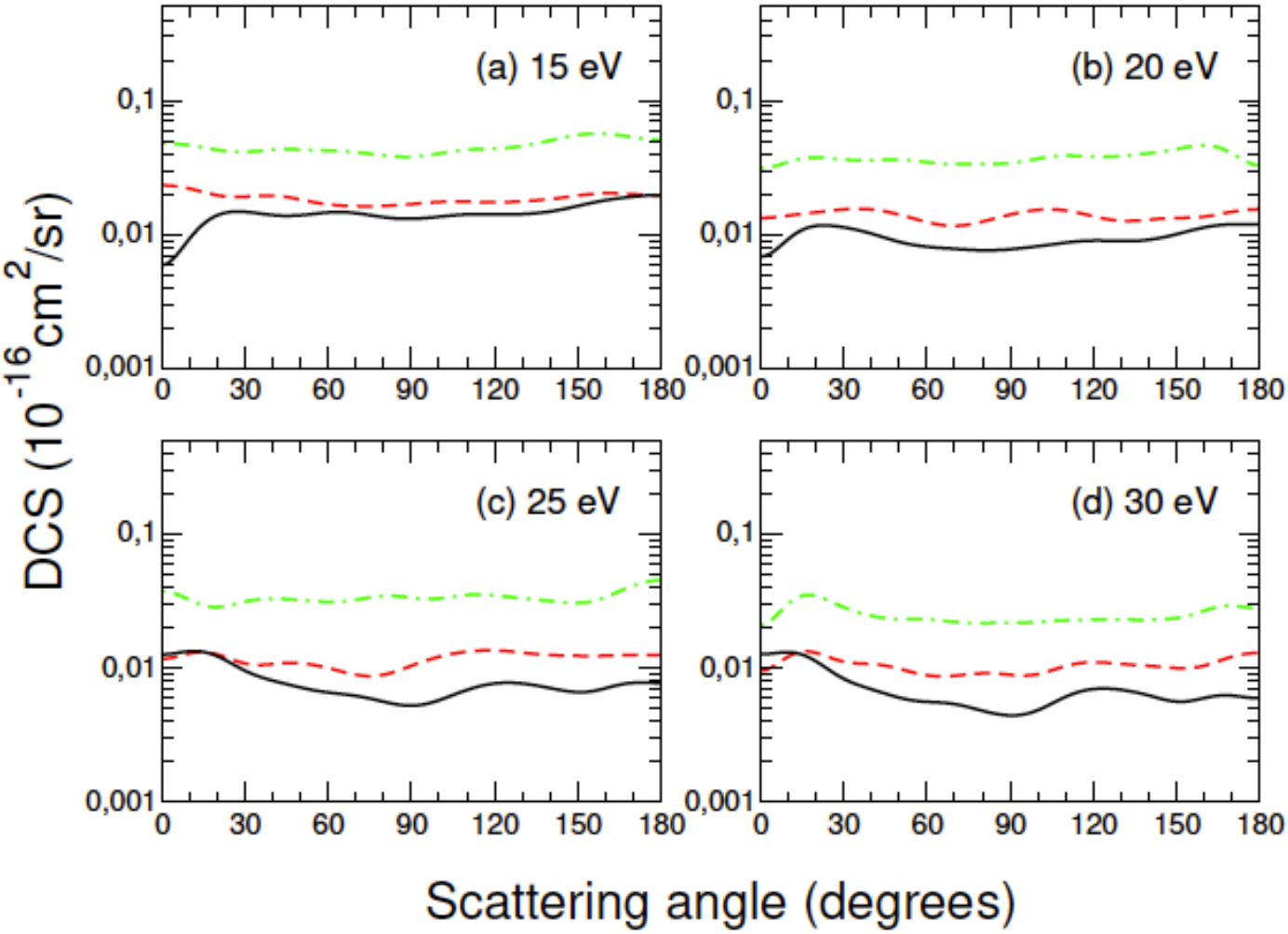


FIG. 3. Differential cross sections (DCS) obtained from the scattering amplitude given by Eq. (1) for the excitation from ground state to the first triplet state ($^3B_{1u}$) of pBQ at the impact energies of (a) 15 eV, (b) 20 eV, (c) 25 eV and (d) 30 eV. Dash-dotted (green) line: 11ch-SEP; dashed (red) line: 38ch-SEP; full (black) line: 89ch-SEP.

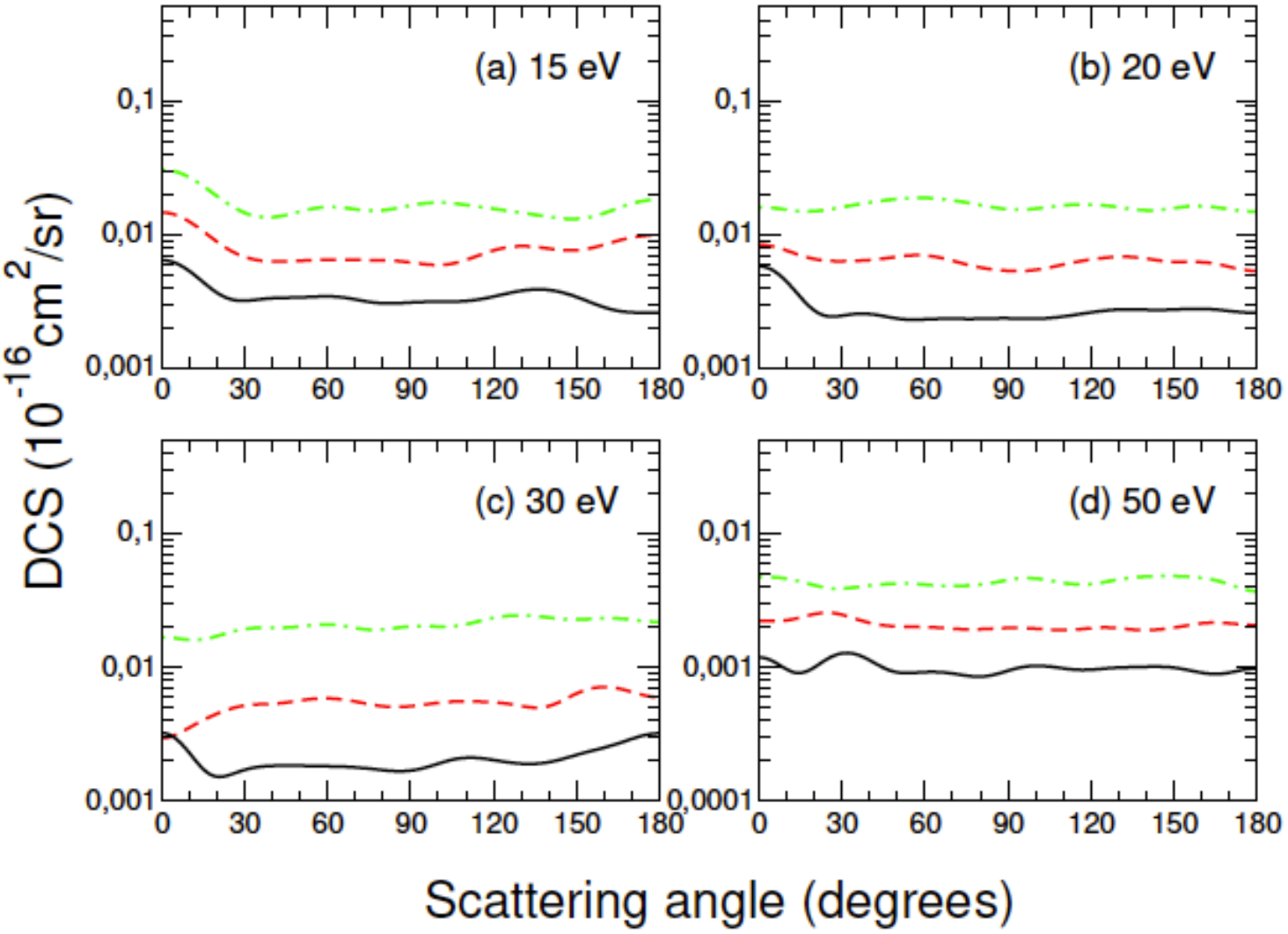


FIG. 8. Differential cross sections (DCS) obtained from the scattering amplitude given by Eq. (1) for the excitation from ground state to the first singlet state ($^1B_{1g}$) of pBQ at the impact energies of (a) 15 eV, (b) 20 eV, (c) 30 eV and (d) 50 eV. Dash-dotted (green) line: 11ch-SEP; dashed (red) line: 38ch-SEP; full (black) line: 89ch-SEP.

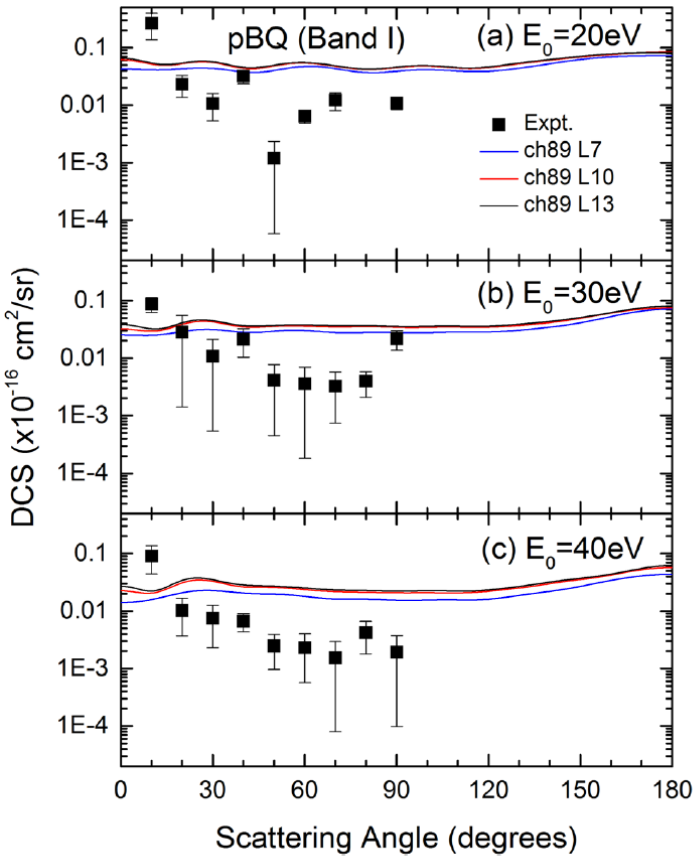


FIG. 3. Experimental and theoretical differential cross sections for electron impact excitation of composite electronic band I ($E_L \sim 4.38$ eV) of pBQ at impact energies of (a) $E_0 = 20$ eV, (b) $E_0 = 30$ eV, and (c) $E_0 = 40$ eV. See the legend in the figure and text for further details.

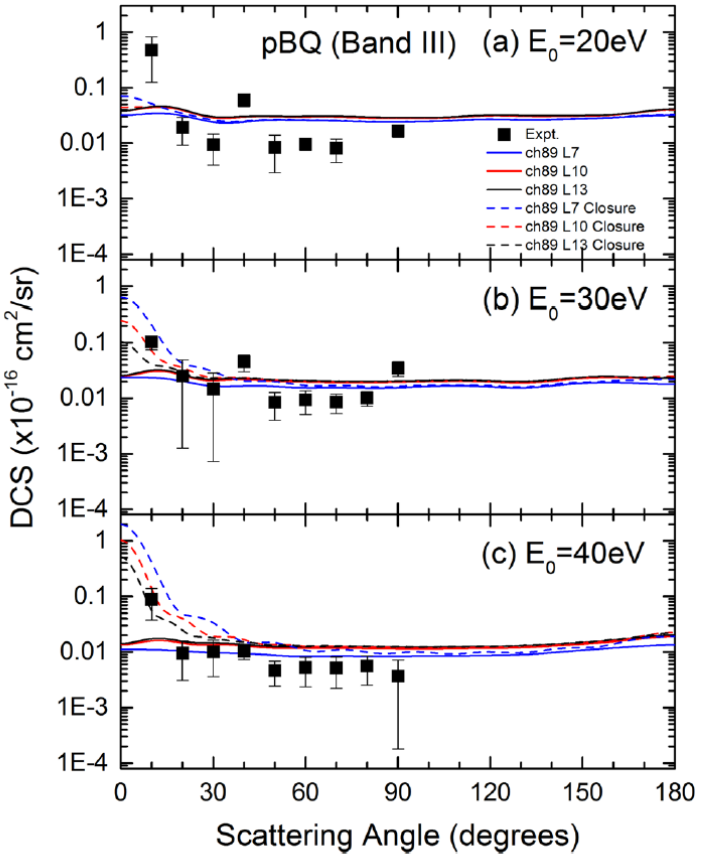


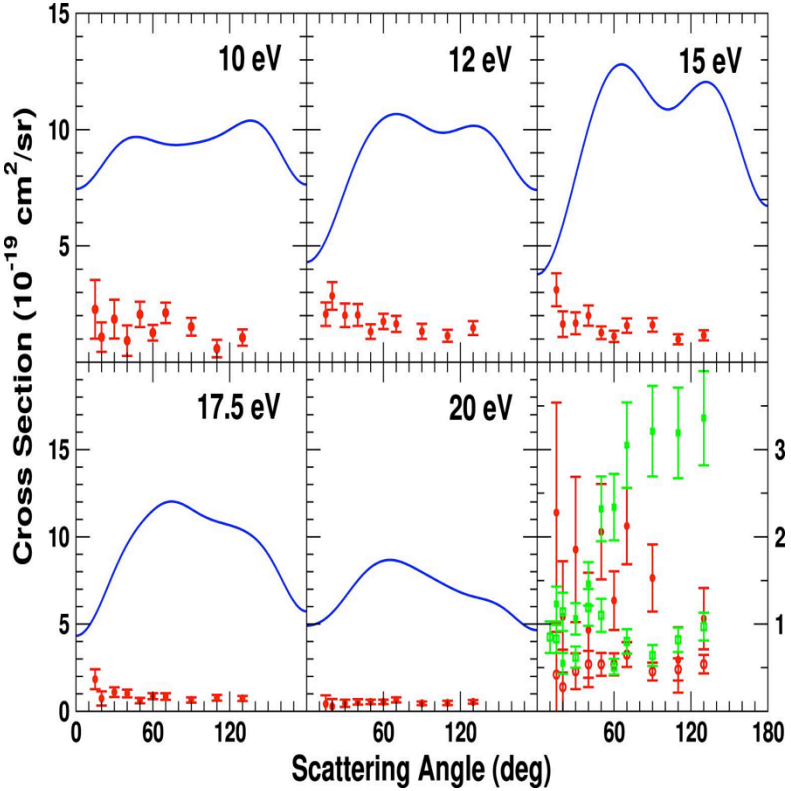
FIG. 5. Experimental and theoretical differential cross sections for electron impact excitation of composite electronic band III ($E_L \sim 6.4$ eV) of pBQ at impact energies of (a) $E_0 = 20$ eV, (b) $E_0 = 30$ eV, and (c) $E_0 = 40$ eV. See the legend in the figure and text for further details.

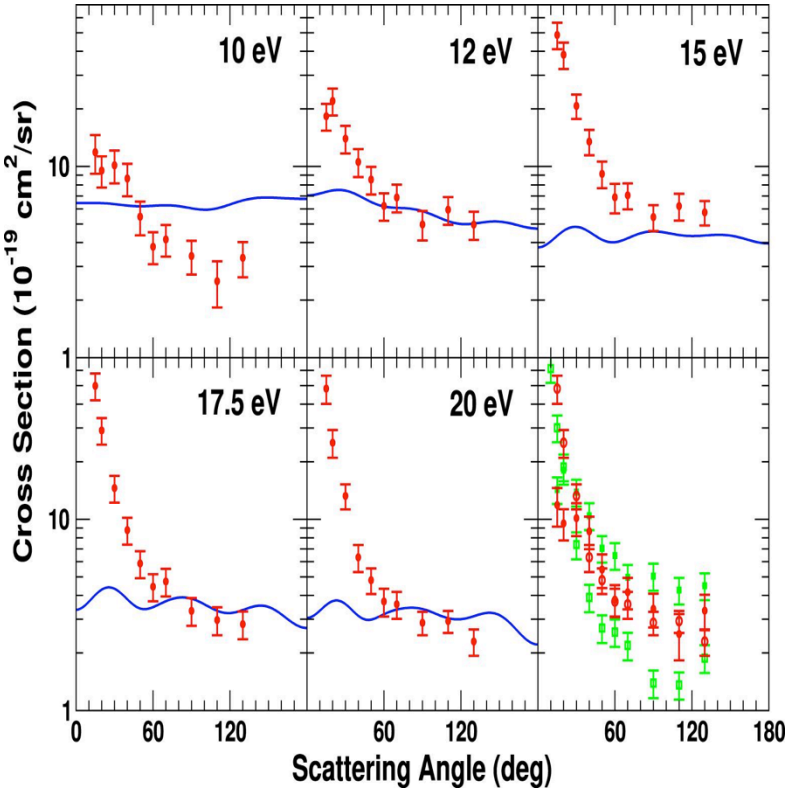
ELECTRONIC EXCITATION – Back to Ethanol

Alan G. Falkowski, Marco A. P. Lima and Fabris Kossoski: a new look at electron-ethanol scattering

First: existing results

I ^{3}A" (left) and I ^{1}A" (right) for trans conformer





L. R. Hargreaves, M. A. Khakoo, C. Winstead, V. McKoy. J. Phys. B: At. Mol. Opt. Phys., 49, 185201 (2016).

Recent implementations on the SMCPP code

(Fábris Kossoski, Aix Marseille University)

- More efficient loops
- Vectorization
- Less I/O
- More specific routines (fewer if-clauses)
- Memory allocation: denominator or off-shell is kept in memory, depending on calculation
- Checkpoints (important for many channels)

Recent implementations on the SMCPP code

(Fábris Kossoski, Aix Marseille University)

Benchmark for CH_3Cl	Before	Now
Elastic	20h	10h
9 channels, 11 excitations	100h	50h
9 channels, 267 excitations	350h	50h

- Computational time reduced to 10-50 %
- No longer scales with the number of excitations

Alan G. Falkowski (master thesis project), Marco A. P. Lima and Fabris Kossoski

Computational aspects (newer version of the parallel SMCPP computer code developed by Fabris Kossoski)

Geometry optimization:
Restricted Hartree-Fock (RHF) with aug-cc-pVDZ and MP2 in GAMESS.

Electronic ground state:
RHF, with *5s5p2d* set, diffuse functions (*1s1p1d*) in C and O.
For the H atoms (*4s/3s*), with addition of one *p* function.
Pseudopotentials BHS.

Ground state and excited states → **Target description in scattering**

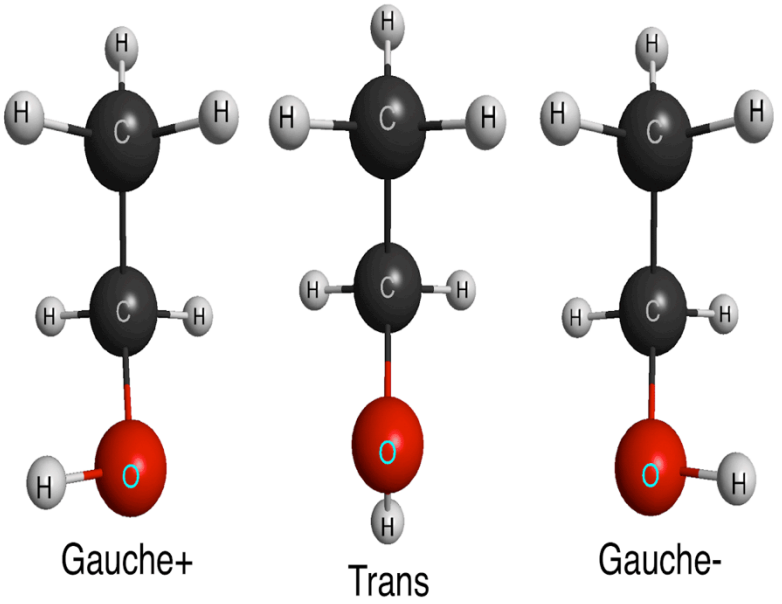
Excited states

IVOs of singlet multiplicity → MOB-SCI with the criterion of the weighted sum*

Multichannel scattering: SMCPP method.

Trans (C_S): 11, 41, 183, 317 and 431 open channels below 10 eV, 12 eV, 15 eV, 17.5 eV and 20 eV

Gauche (C_1): 183 open channels bellow 15 eV.



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New strategy allows a "densification" of the open channels bellow ϵ_{open}

# Hole-particle pairs\ϵ_{open}	10 (10.5) eV	12 eV	15 eV	17.5 eV	20 eV
5	10				
20	12	40			
91	14	55	182		
158	15	59	222	316	
215	15	59	224	367	430
FCIS (1520)	18	63	239	398	544

Number of open excited states (singlet + triplets)

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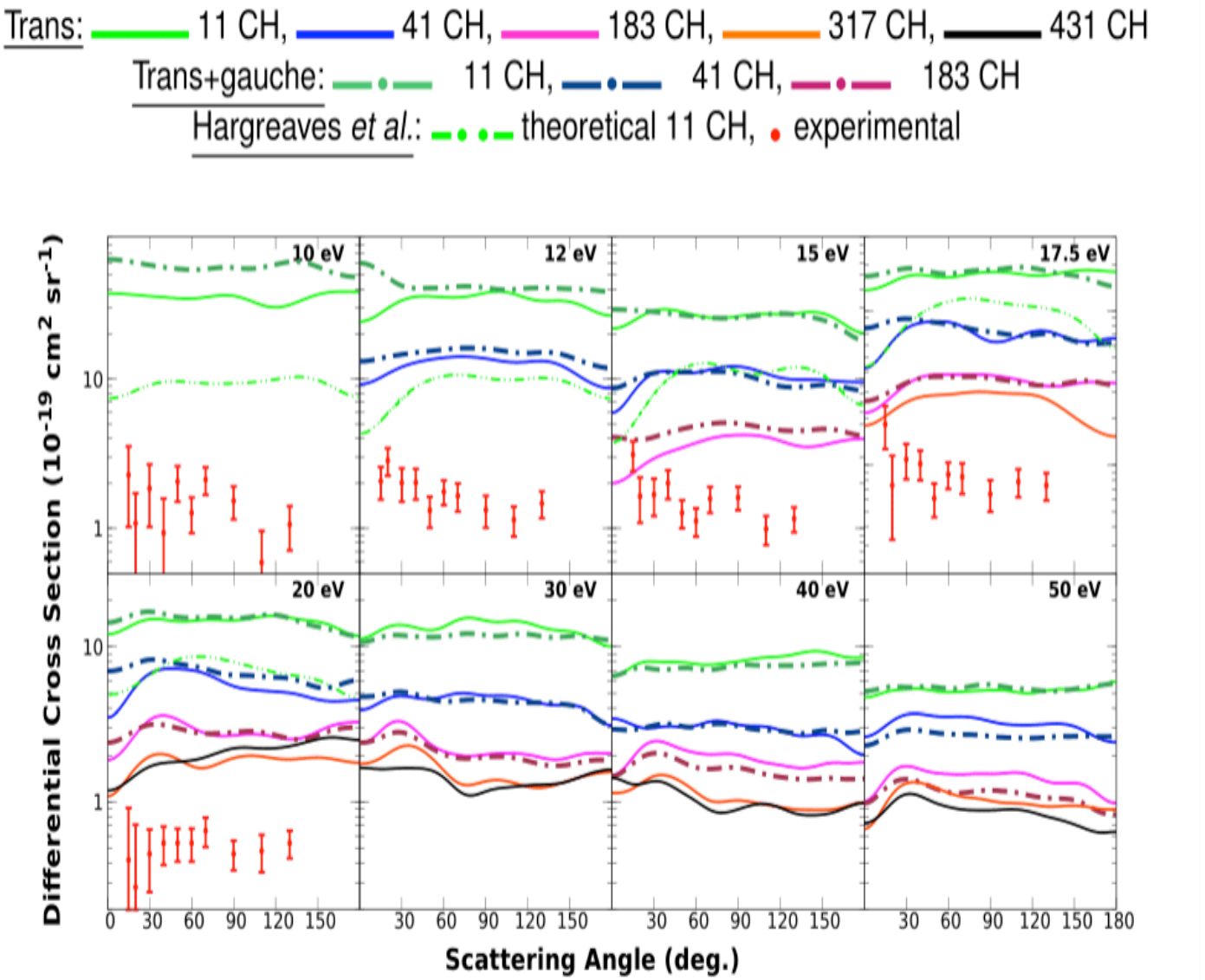
Marco A. P. Lima and Fabris Kossoski

Results: I $^3A"$



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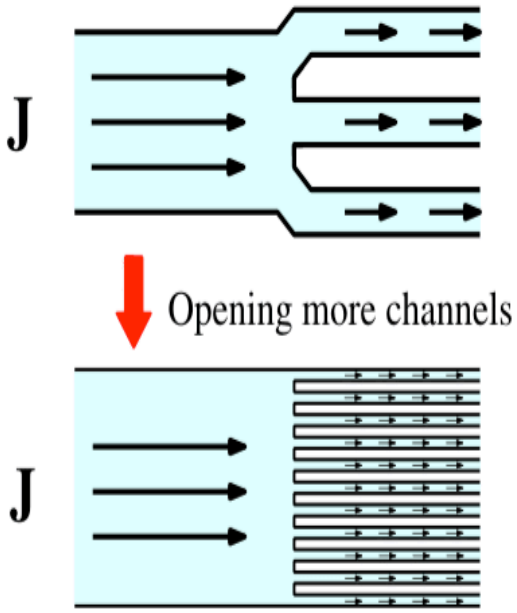
Flux competition

$$\frac{d\sigma}{d\Omega} \propto |\mathbf{J}| \text{ (Probability current)}$$

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{J} = 0, \qquad \mathbf{J} = \frac{\hbar^2}{2mi} \mathrm{Re}\{\Psi^* \nabla \Psi\}$$



*Observed in the previous studies of our group.

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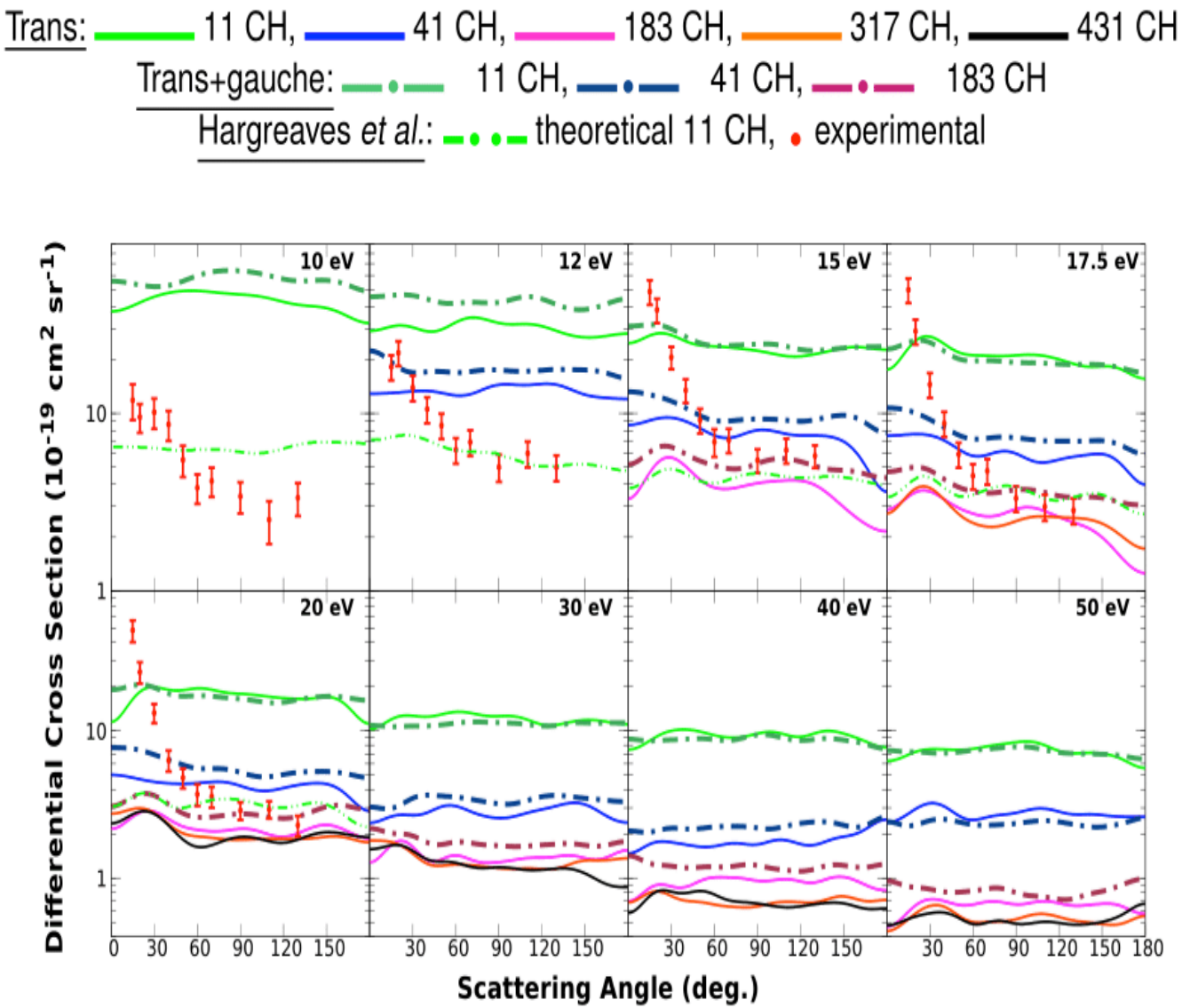
Results: I ¹A"



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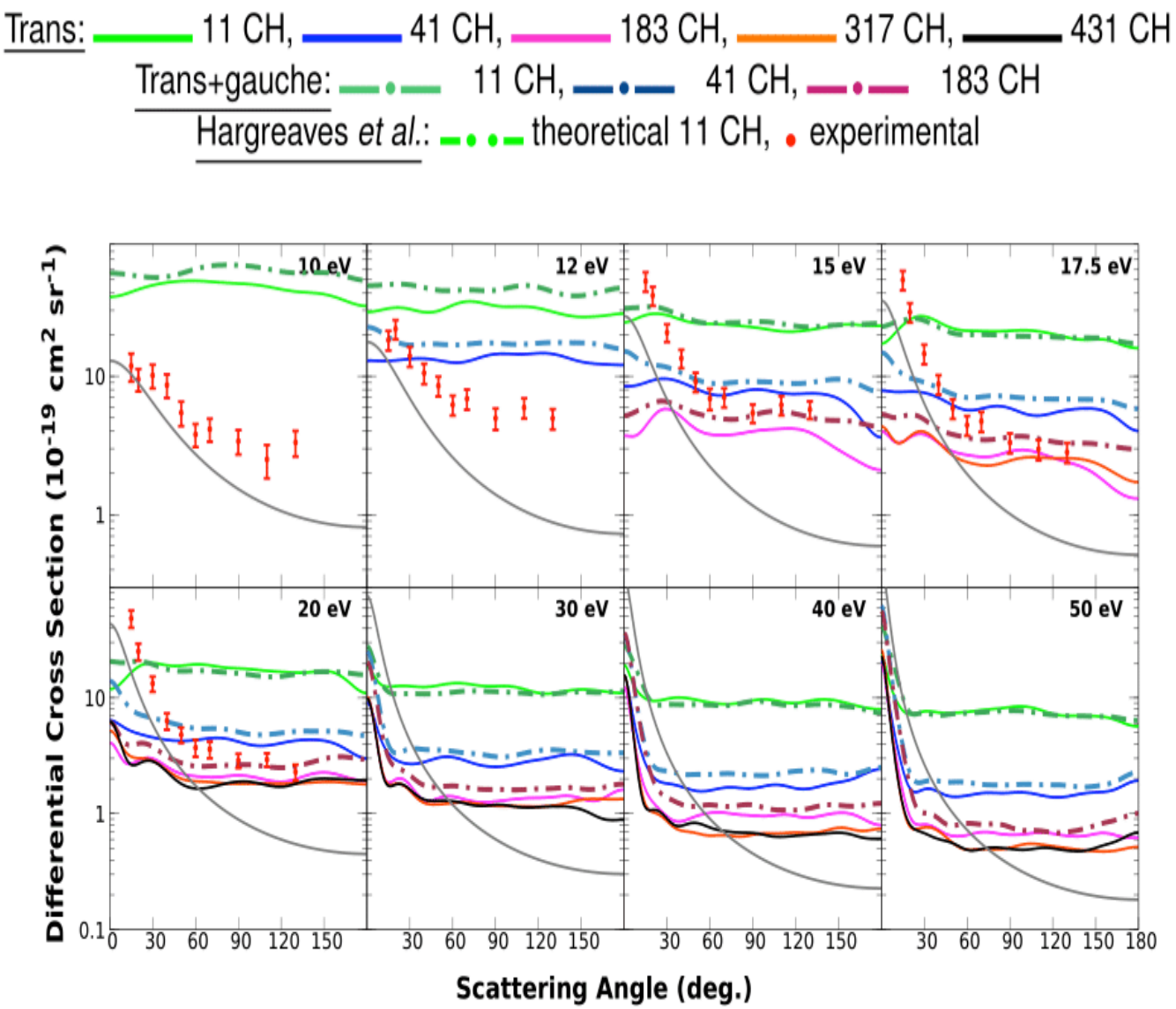
Results: I [A" with Born-closure



We will review smaller systems and explore the limits of the new strategy.

Thank you for your attention