Calculation of Atomic and Molecular Collisions

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Motivation

The primary motivation is to provide accurate atomic and molecular collision data for science and industry

- Astrophysics
- Fusion research
- Fluorescent lighting
- Nanolithography
- Neutral antimatter formation
- Medical: cancer imaging and therapy

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Challenges

Collisions between particles on the atomic scale are difficult to calculate:

- Governed by the Laws of Quantum Mechanics
  1. Countably infinite discrete target spectrum
  2. Uncountably infinite target continuum
  3. Charged particles interact at infinite distances
- Close-coupling bypasses these problems!
  1. Finite number of square-integrable target states
  2. Unitary excitation of $-$ve- and $+$ve-energy states
  3. Effectively, only one charged particle at infinity

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Convergent close-coupling theory

Target structure

Use complete Laguerre basis $\xi_{n\ell}^{(\lambda)}(r) \propto \exp(-\lambda_\ell r)$:

- "one-electron" (H, Ps, Li,. . . ,Cs, H_2^+)

$$\phi_{n\ell}(r) = \sum_{n'=1}^{N_\ell} C_{n\ell}^{n'} \xi_{n'\ell}^{(\lambda)}(r),$$

- "two-electron" (He, Be,. . . , Hg, Ne, . . . , Xe, H_2, H_2O)

$$\phi_{n\ell s}(r_1, r_2) = \sum_{n',n''} C_{n\ell s}^{n'n''} \xi_{n'\ell'}^{(\lambda)}(r_1) \xi_{n''\ell''}^{(\lambda)}(r_2),$$

- Diagonalise the target (FCHF) Hamiltonian

$$\langle \phi_f | H_T | \phi_i \rangle = \varepsilon_f \delta_{fi}, \quad i, f = 1, \ldots, N$$

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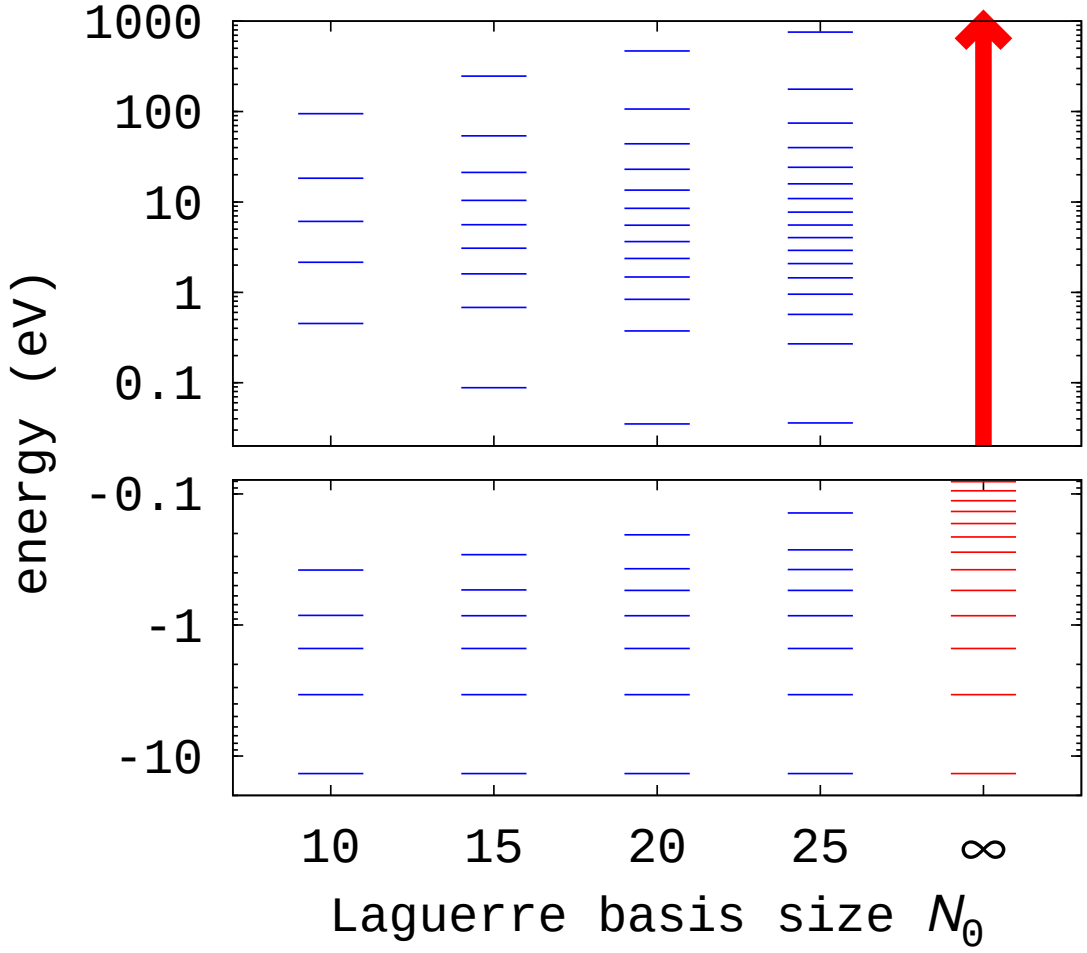
Target structure

- H s-state energies for Laguerre bases N_0 with $\lambda_0 = 1$



- $I_{N_\ell} = \sum_{n=1}^{N_\ell} |\phi_{n\ell}\rangle\langle\phi_{n\ell}|, \quad \lim_{N_\ell\to\infty} I_{N_\ell} = I_\ell.$

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Electron scattering

- Electron-atom/molecule wavefunction:

$$|\Psi_i^{(+)}\rangle \approx \mathcal{A} I_N |\psi_i^{(+)}\rangle = \mathcal{A} \sum_{n=1}^{N} |\phi_n F_{ni}\rangle. \tag{1}$$

  - $\mathcal{A}$ leads to non-uniqueness of F_{ni}
- Solve for $T_{fi} \equiv \langle \boldsymbol{k}_f \phi_f | V | \Psi_i^{(+)} \rangle$ at $E = \varepsilon_i + {k_i}^2/2$,

$$\langle \boldsymbol{k}_f \phi_f | T | \phi_i \boldsymbol{k}_i \rangle = \langle \boldsymbol{k}_f \phi_f | V | \phi_i \boldsymbol{k}_i \rangle + \sum_{n=1}^{N} \int d^3k \frac{\langle \boldsymbol{k}_f \phi_f | V | \phi_n \boldsymbol{k} \rangle \langle \boldsymbol{k} \phi_n | T | \phi_i \boldsymbol{k}_i \rangle}{E + i0 - \varepsilon_n - k^2/2}. \tag{2}$$

  - $\lim_{N\to\infty} \langle \boldsymbol{k}_f \phi_f | T | \phi_i \boldsymbol{k}_i \rangle = 0$ for $k_f^2/2 < \varepsilon_f$ i.e. $\epsilon_f > E/2$.
- Excitation: $\sigma_{fi} \equiv \frac{k_f}{k_i} |\langle \boldsymbol{k}_f \phi_f | T | \phi_i \boldsymbol{k}_i \rangle|^2$, $\varepsilon_f < 0$
- Ionization: $\sigma_{fi} \equiv |\langle \boldsymbol{q}_f^{(-)} | \phi_f \rangle \langle \boldsymbol{k}_f \phi_f | T | \phi_i \boldsymbol{k}_i \rangle|^2$, $0 < \varepsilon_f \leq \frac{E}{2}$

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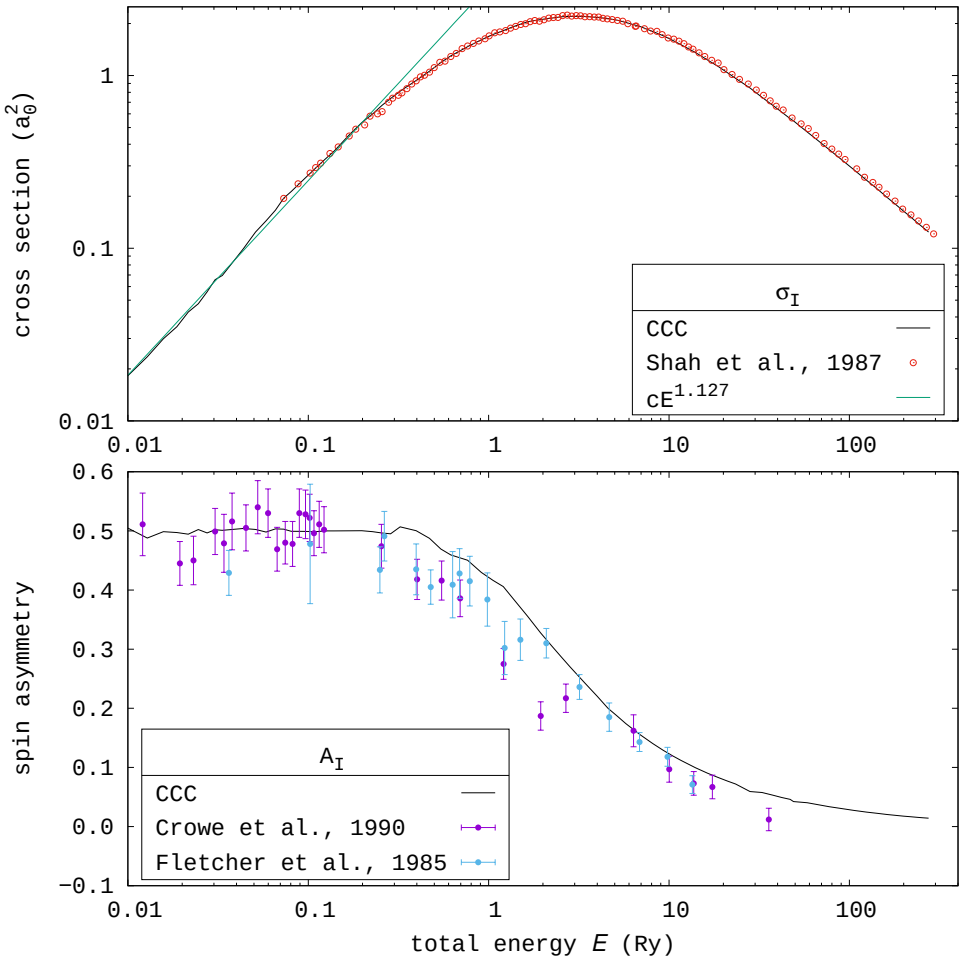
Electron scattering on atomic hydrogen

- e^--H total ionization cross section and spin asymmetry



[I. Bray *et al.*, PRL **121**, 203401 (2018)]

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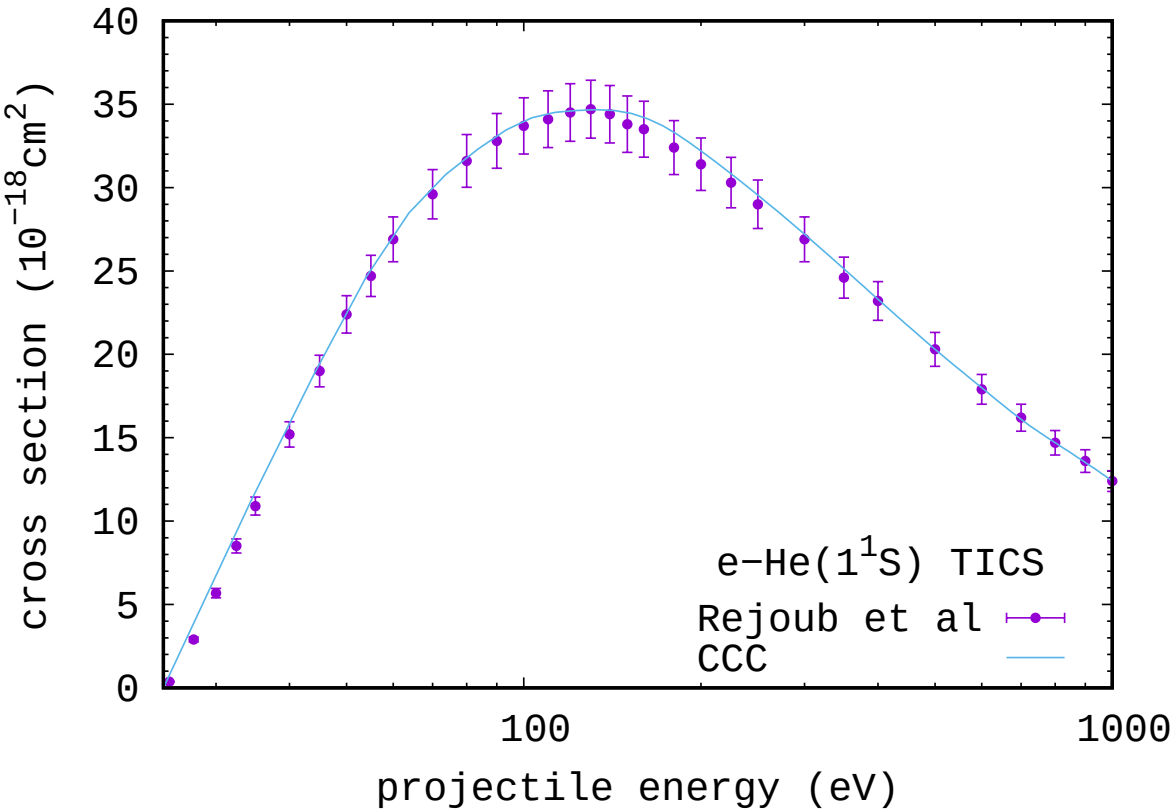
Electron scattering on He(1^1S)

- e^--He(1^1S) total ionization cross section



[Bray and Fursa, JPB **44**, 061001 (2011)]

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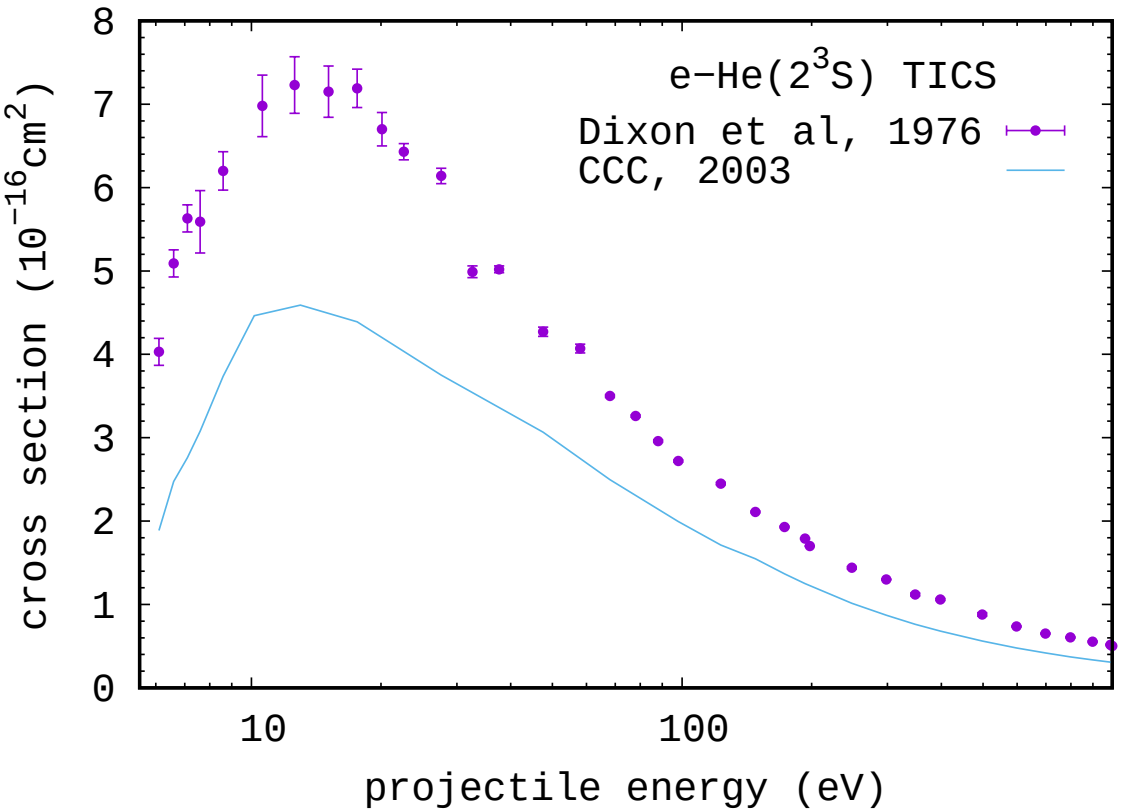
Electron scattering on He(2^3S)

- e^--He(2^3S) total ionization cross section



[Fursa and Bray, JPB **36**, 1663 (2003)]

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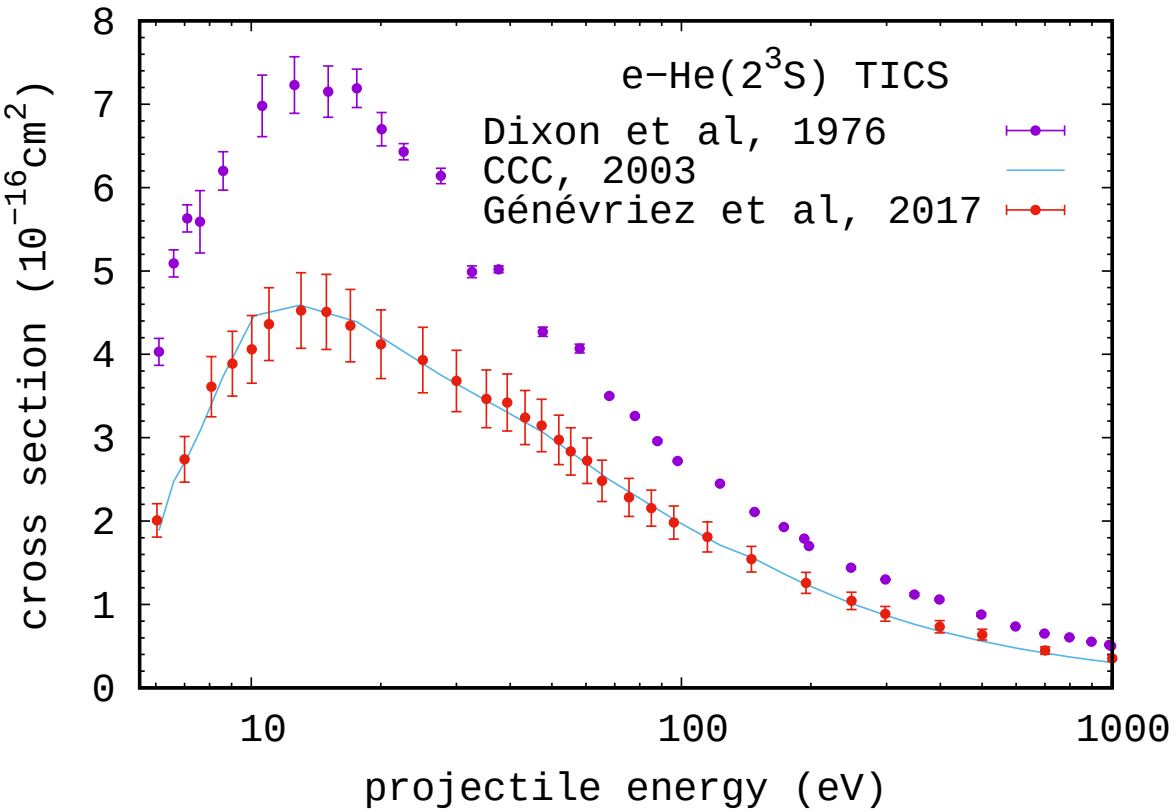

[Génévriez *et al.*, PRA **96**, 010701(R) (2017)]

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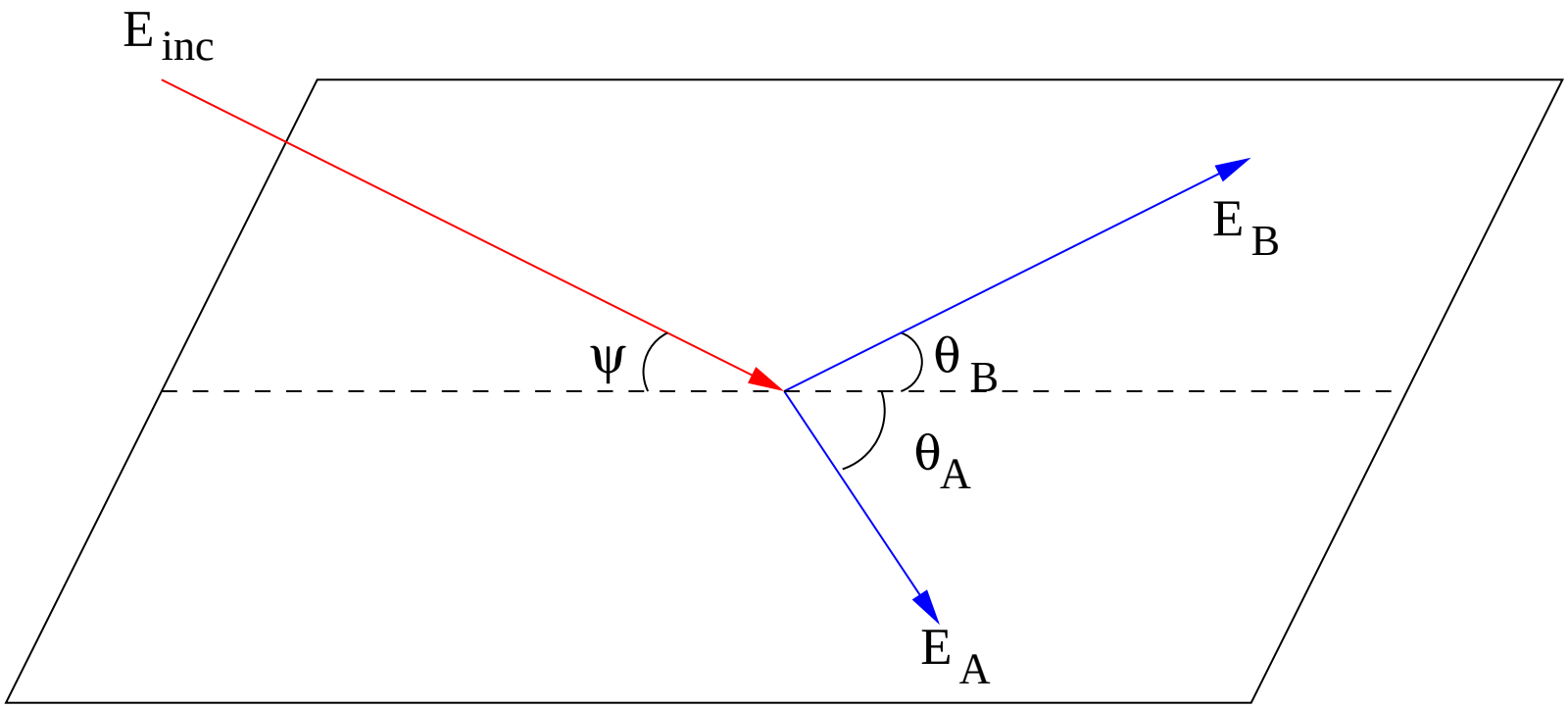
Fully differential ionization geometry



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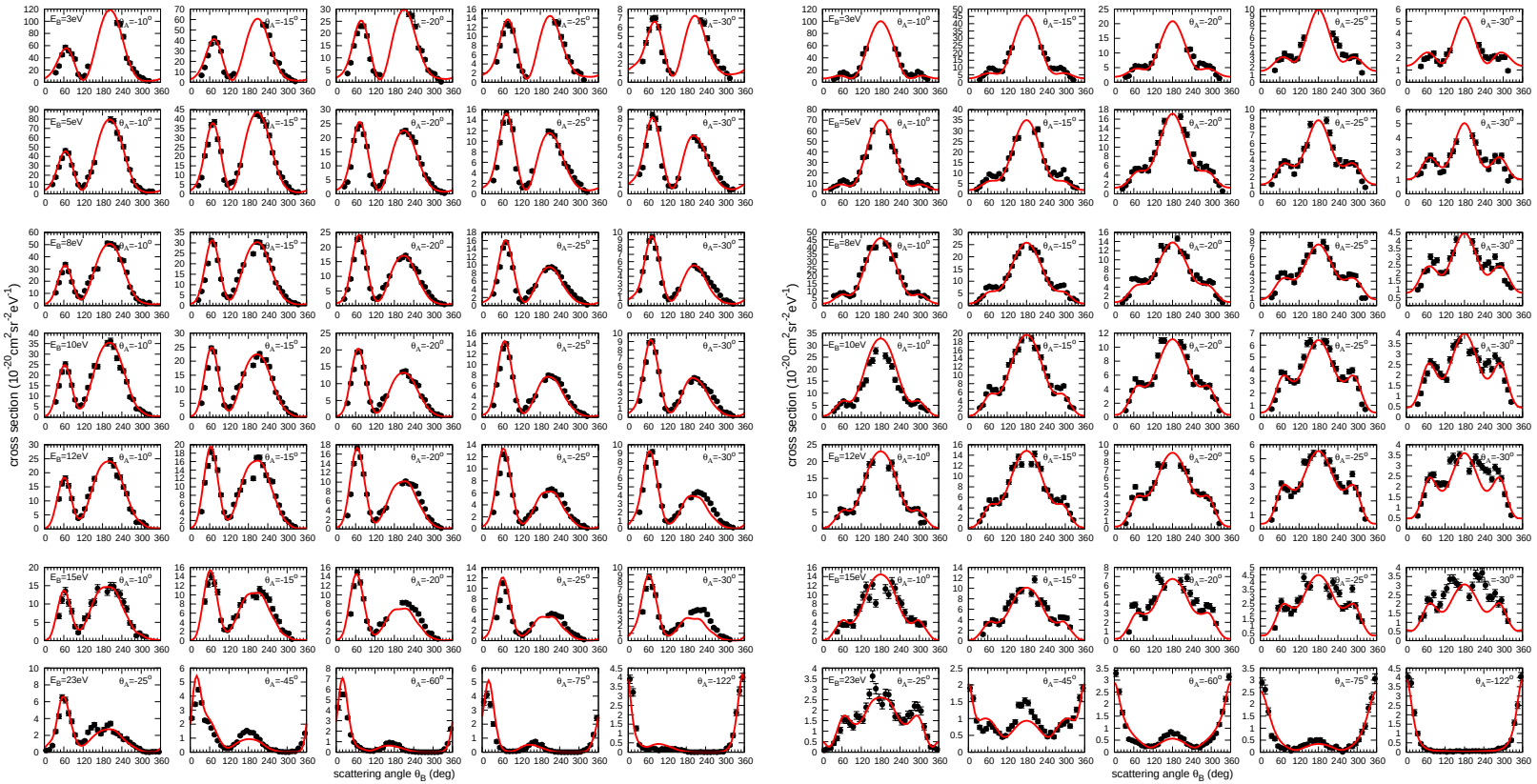
71 eV e^--He fully differential single ionization



[X. Ren *et al.*, PRA **83**, 052711 (2011)]

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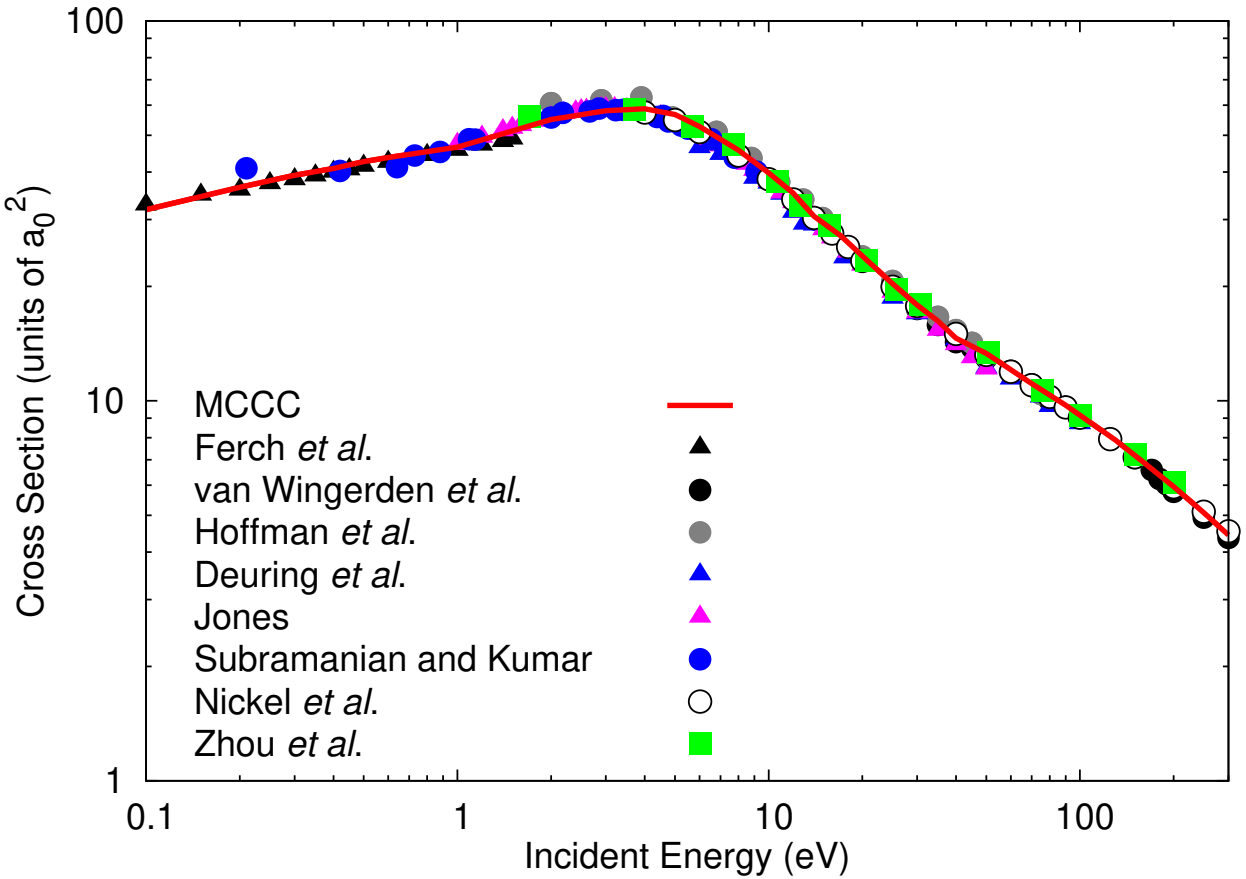
Electron scattering on molecular hydrogen

- e^--H_2 collisions: MCCC-calculated total cross section



[M. Zammit *et al.*, PRL **116**, 233201 (2016)]

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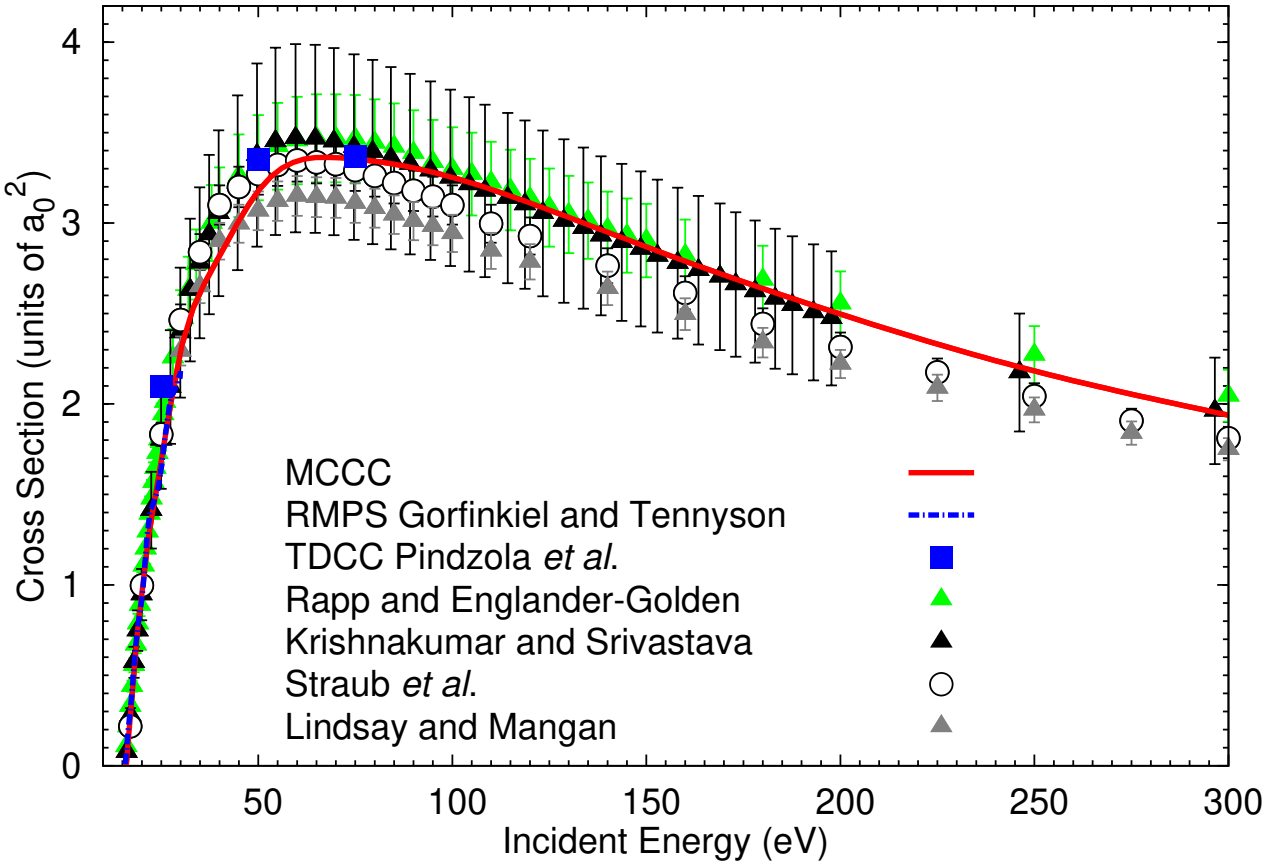

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Electron scattering on molecular hydrogen

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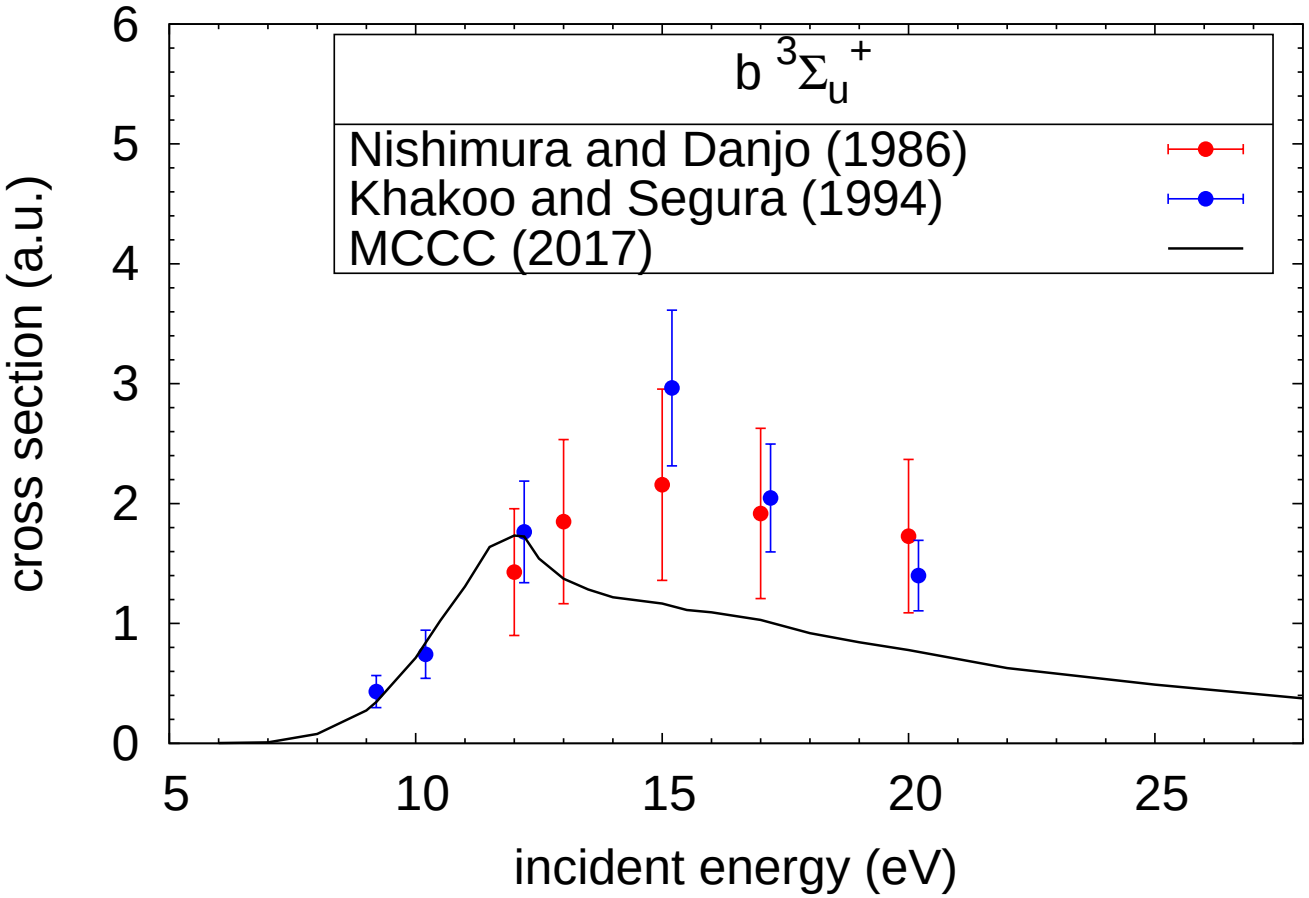

[Zammit *et al.*, PRA **95**, 022708 (2017)]

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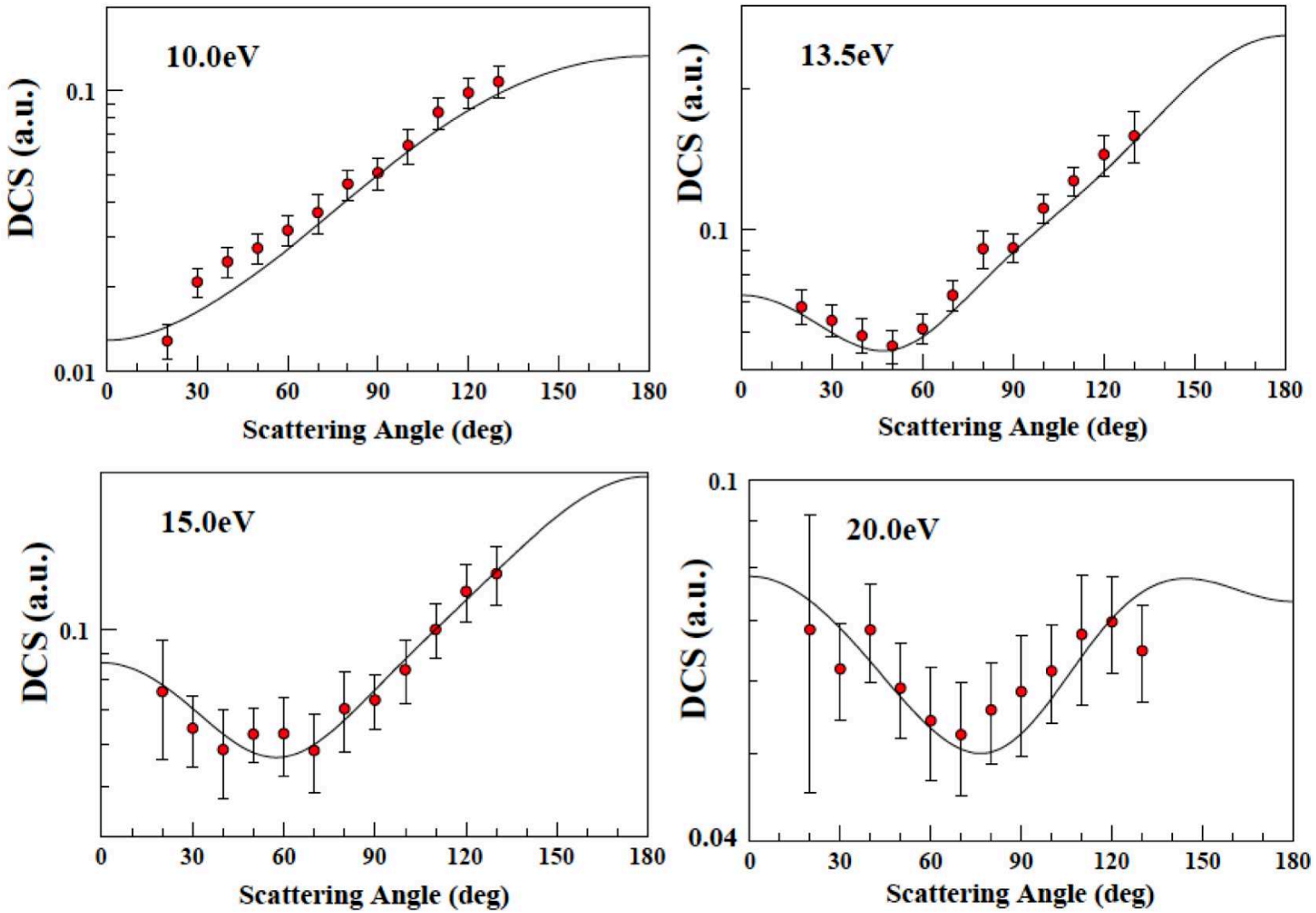

[Zawadski *et al.*, PRA **97** 050702(R) (2018)]

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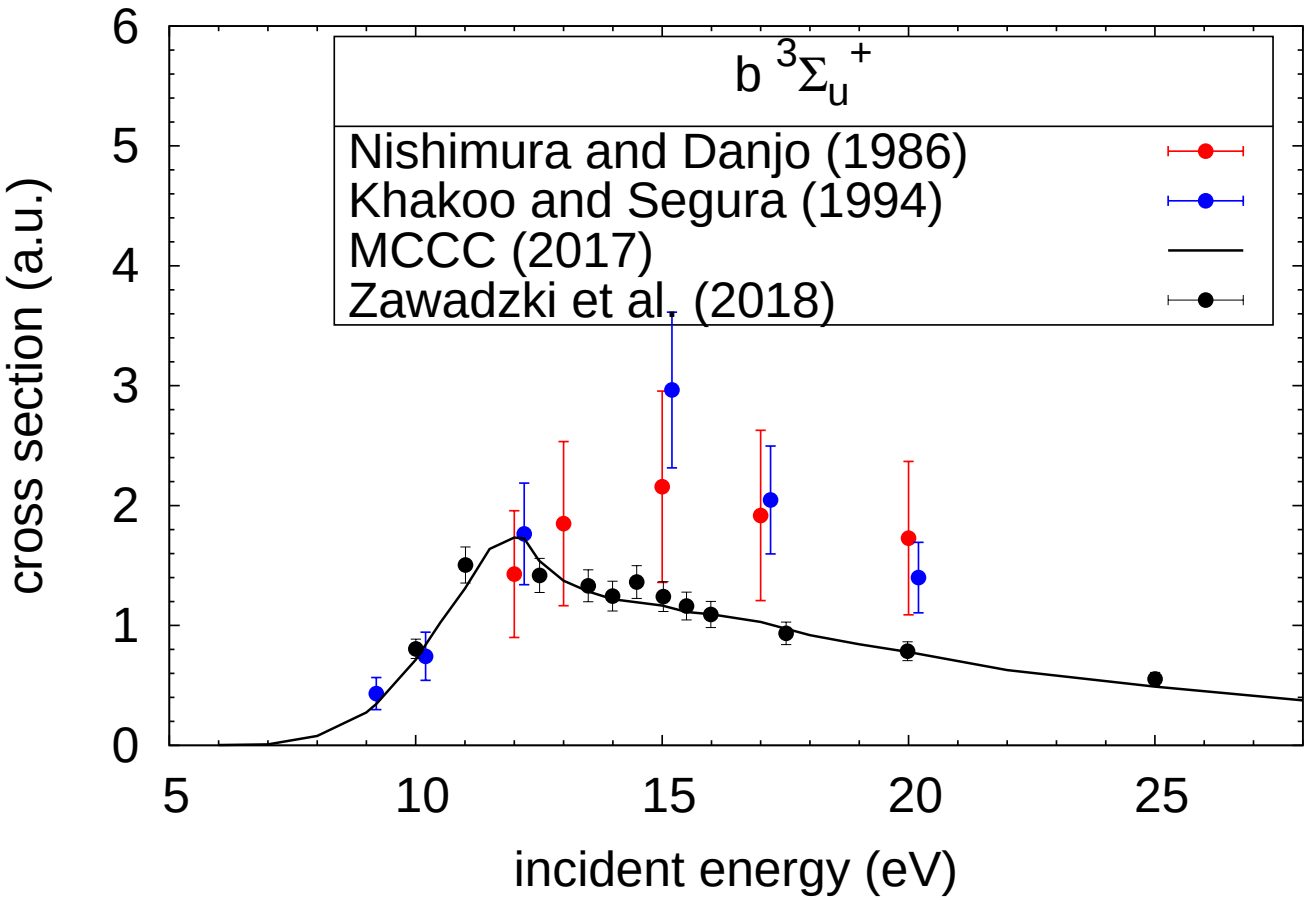

[M. Zawadski *et al.*, PRA **98**, 050702R (2018)]

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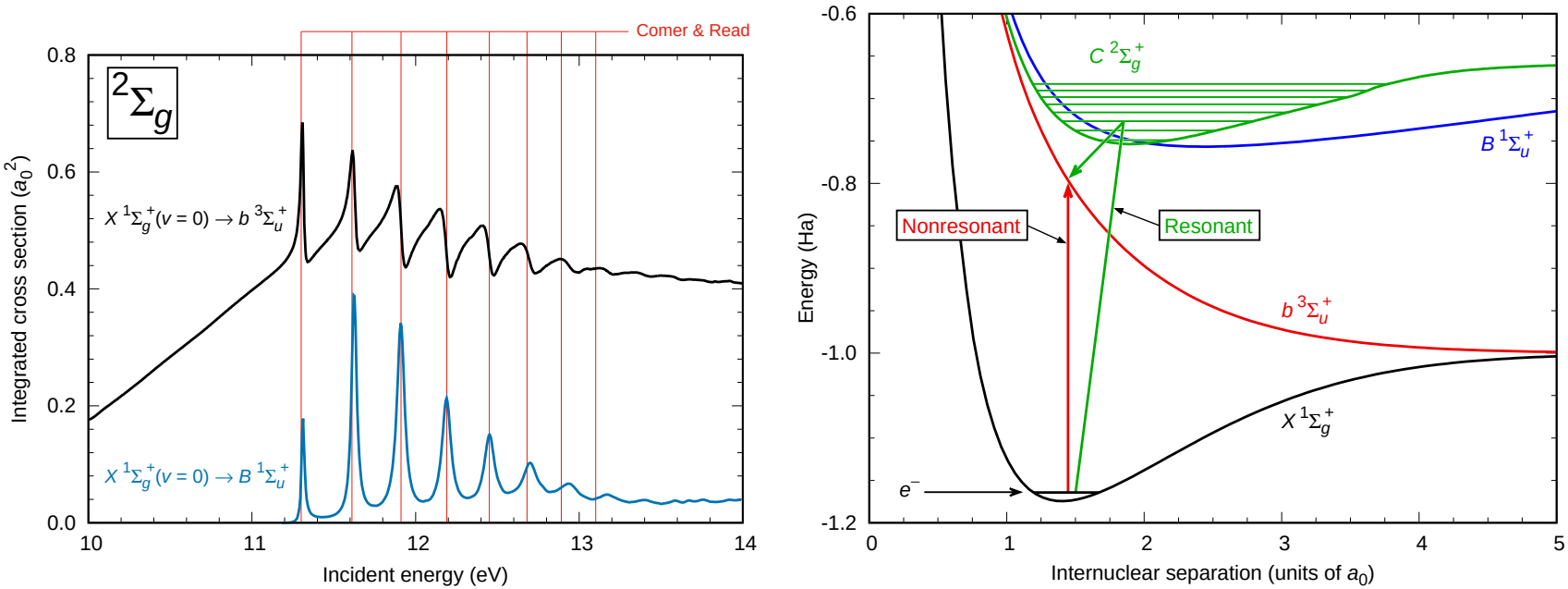
Vibrational-Electronic MCCC

- e^--$H_2(X^1\Sigma_g^+)$ excitation in the $^2\Sigma_g$ symmetry



[Scarlett *et al.*, PRL **127** 223401 (2021)]

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Concluding remarks

- CCC valid at all energies for (anti)electrons, photons, (anti)protons scattering on quasi one- and two- electron atoms and molecules, as well as inert gases.
- Atomic CCC available: https://amosgateway.org.
- Data available: LXCAT, mccc-db.org, CCC-WWW.

To-do list

- Implementing general structure code of Zatsarinny; e^+-C [Mori *et al.* PRA **107** 032817 (2023)]
- Quasi one- and two-electron hydrides LiH, LiH^+, BeH^+; HeH^+ [Scarlett *et al.* PRA **106** 042818 (2022)]
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