Benchmark calculations for electron scattering on atomic hydrogen and helium

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Outline

Introduction
Motivation

- The primary motivation is to provide accurate atomic collision data for science and industry:
  - Astrophysics
  - Fusion research
  - Lighting industry
  - Medical and materials applications
- Provide a rigorous foundation for collision theory with long-ranged (Coulomb) potentials.

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Distant history

- Prior to the 1990s theory and experiment generally did not agree for:
  - electron-hydrogen excitation or ionisation,
  - electron-helium excitation or ionisation,
  - single or double photoionisation of helium.
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  - Two-body problems
  - Three-body problems
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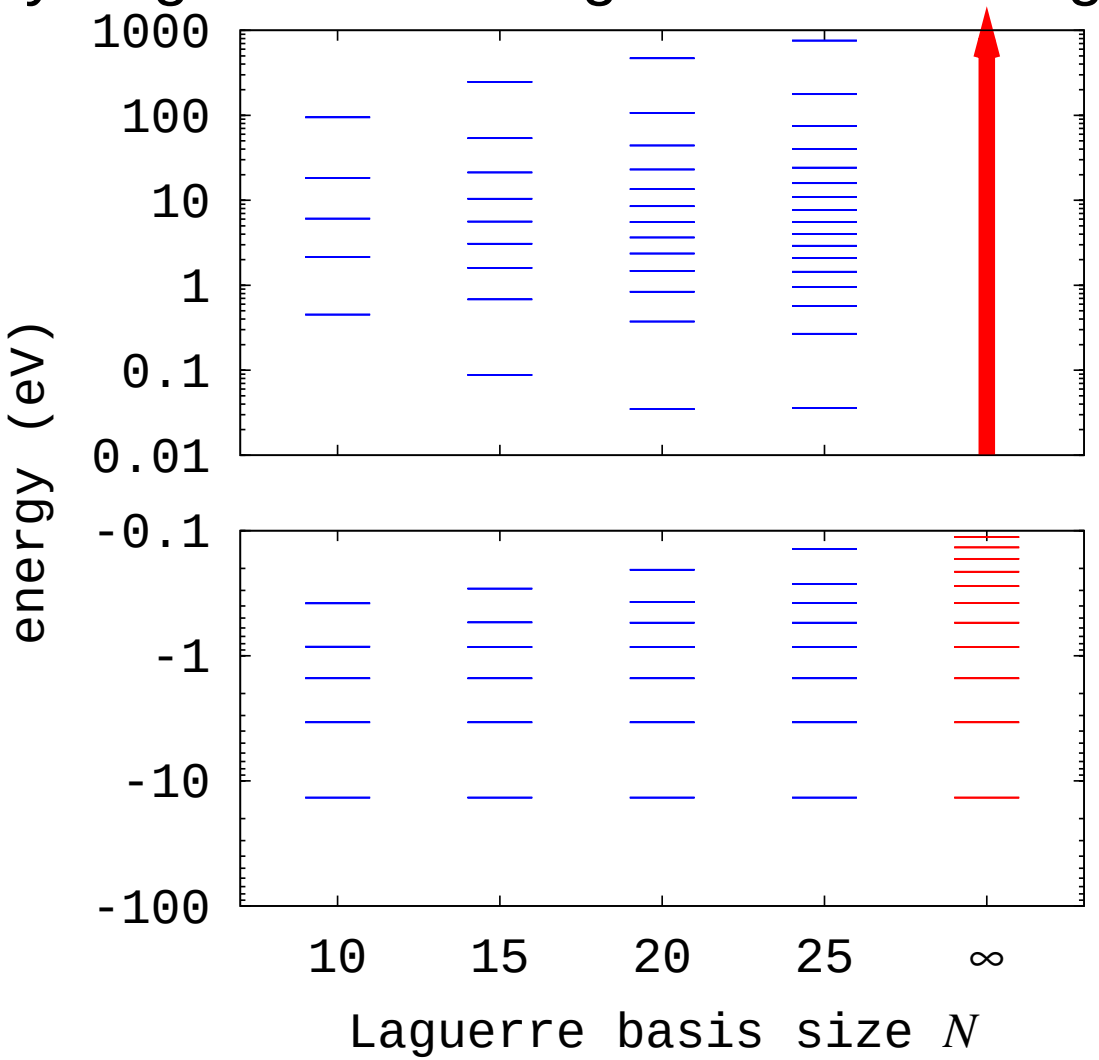
Nonrelativistic CCC theory

target structure and scattering

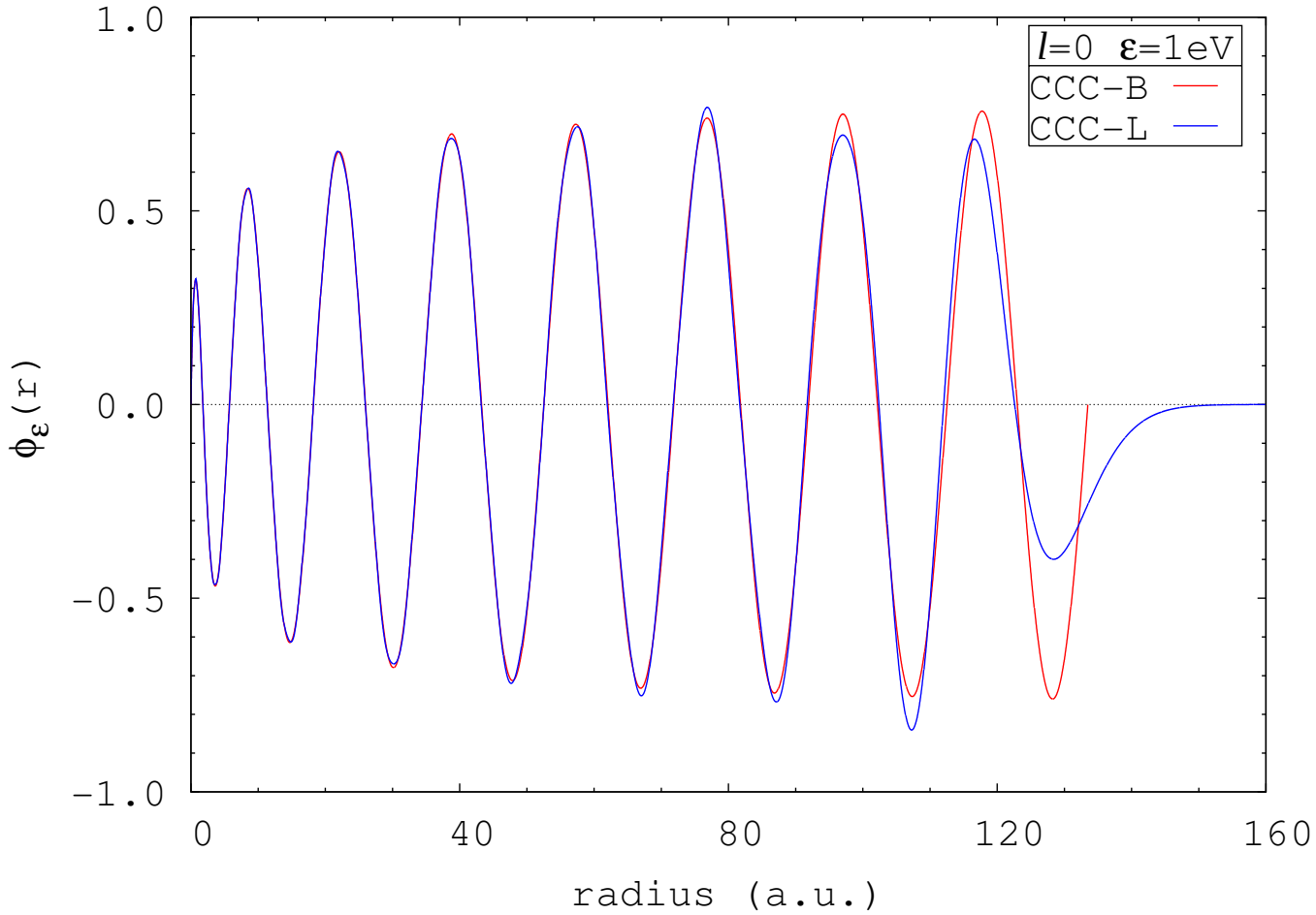
- Structure: using the Laguerre basis $\xi_{nl}^{(\lambda)}(r)$ write:
  - "one-electron" (H, Li, ..., Cs) states:
    $\phi_{nl}^{(\lambda)}(r) = \sum_{n'} C_{nl}^{n'} \xi_{n'l}^{(\lambda)}(r)$
  - "two-electron" (He, Be, ..., Hg) states:
    $\phi_{nls}^{(\lambda)}(r_1, r_2) = \sum_{n',n''} C_{nls}^{n'n''} \xi_{n'l'}^{(\lambda)}(r_1) \xi_{n''l''}^{(\lambda)}(r_2)$.
  - Coefficients C are obtained by diagonalising the target (FCHF) Hamiltonian

$$\langle \phi_f^{(\lambda)} | H_{\rm T} | \phi_i^{(\lambda)} \rangle = \varepsilon_f^{(\lambda)} \delta_{fi}. \qquad (1)$$

- Hydrogen $\ell = 0$ energies for $\lambda = 1$ Laguerre bases



- $\phi_\varepsilon^{(\lambda)}(r)$ for $N = 70, \lambda = 2$ and $\phi_\varepsilon^{(R_0)}(r)$ for $R_0 = 134$.



- Scattering:
  - Electron-atom wavefunction is expanded as

$$|\Psi_i^{(+)}\rangle \approx \mathcal{A}\sum_{n=1}^{N}|\phi_n^{(\lambda)}\rangle\langle\phi_n^{(\lambda)}|\psi_i^{(+)}\rangle \equiv \mathcal{A}I_N|\psi_i^{(+)}\rangle. \quad (2)$$

  - Solve for $T_{fi} \equiv \langle \boldsymbol{k}_f\phi_f^{(\lambda)}|V|\Psi_i^{(+)}\rangle$ at $E = \varepsilon_i^{(\lambda)} + \epsilon_{k_i}$,

$$\langle \boldsymbol{k}_f\phi_f^{(\lambda)}|T|\phi_i^{(\lambda)}\boldsymbol{k}_i\rangle = \langle \boldsymbol{k}_f\phi_f^{(\lambda)}|V|\phi_i^{(\lambda)}\boldsymbol{k}_i\rangle + \sum_{n=1}^{N}\sum\!\!\!\!\!\!\int d^3k\,\frac{\langle \boldsymbol{k}_f\phi_f^{(\lambda)}|V|\phi_n^{(\lambda)}\boldsymbol{k}\rangle\langle \boldsymbol{k}\phi_n^{(\lambda)}|T|\phi_i^{(\lambda)}\boldsymbol{k}_i\rangle}{E + i0 - \varepsilon_n^{(\lambda)} - \epsilon_k}. \quad (3)$$

  - Have step-function behaviour:

$$\langle \boldsymbol{k}_f\phi_f^{(\lambda)}|T|\phi_i^{(\lambda)}\boldsymbol{k}_i\rangle \approx 0 \text{ for } \varepsilon_f^{(\lambda)} > \epsilon_{k_f}.$$

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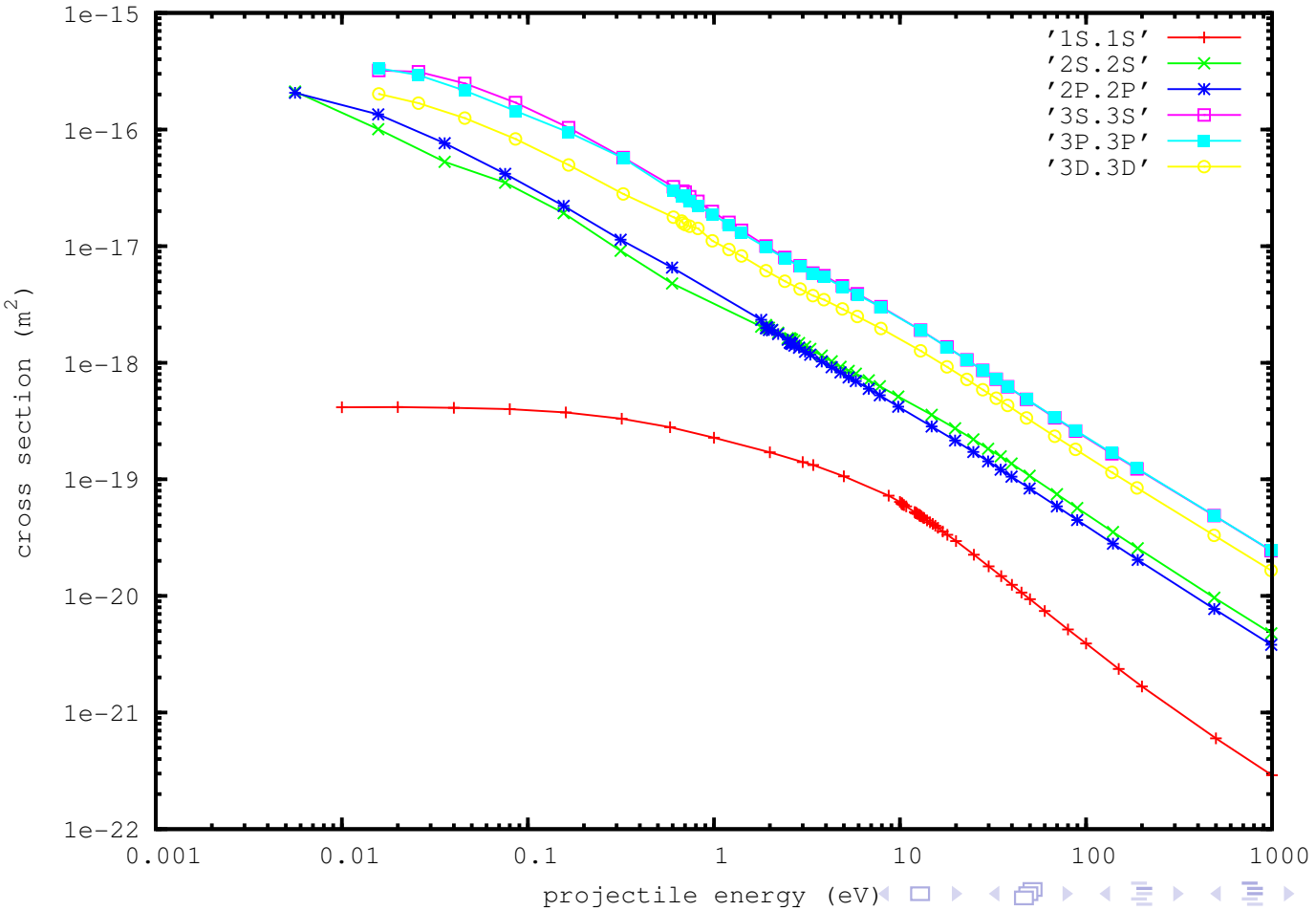
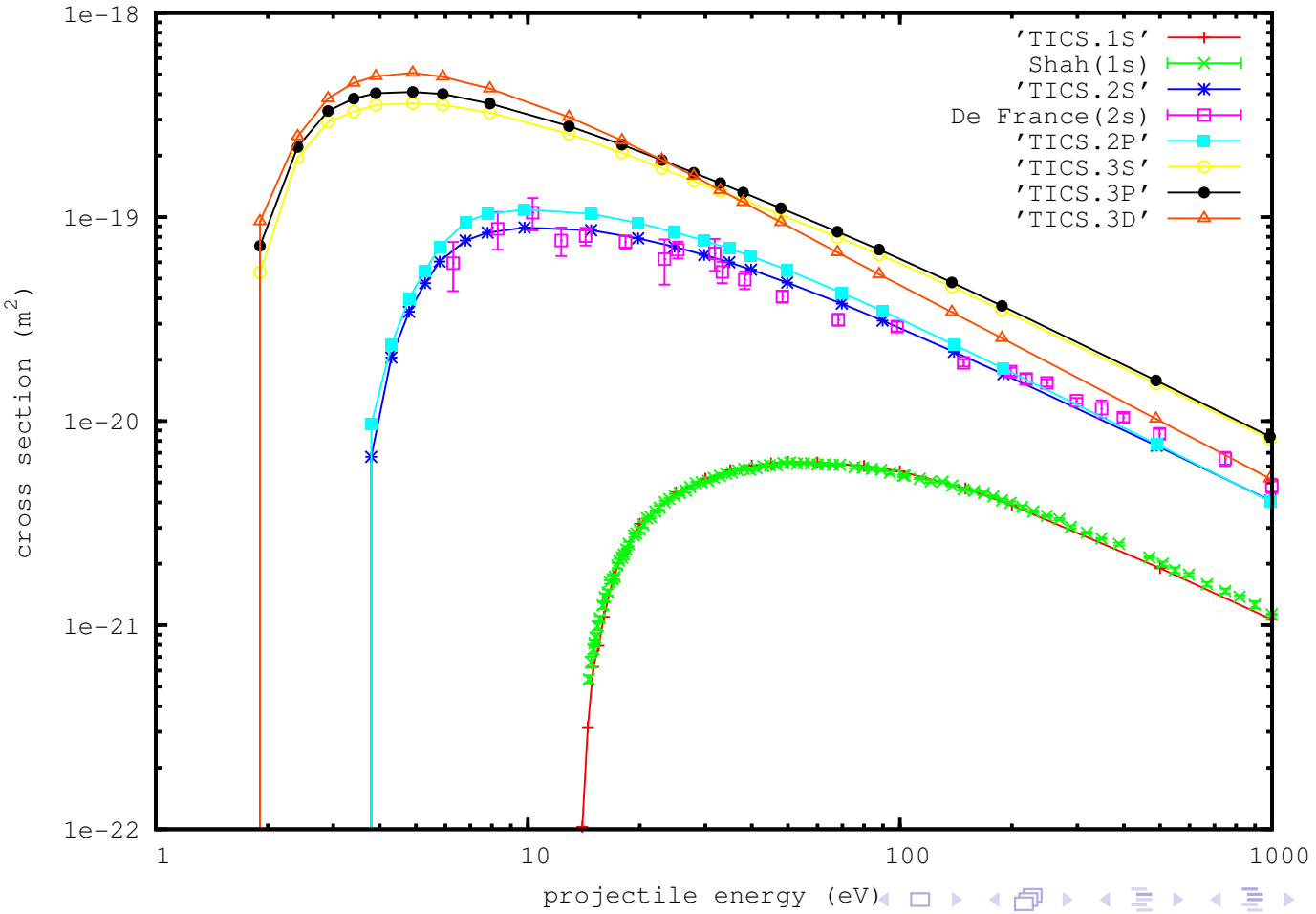
Electron-hydrogen scattering

- elastic scattering for $n \leq 3$ states



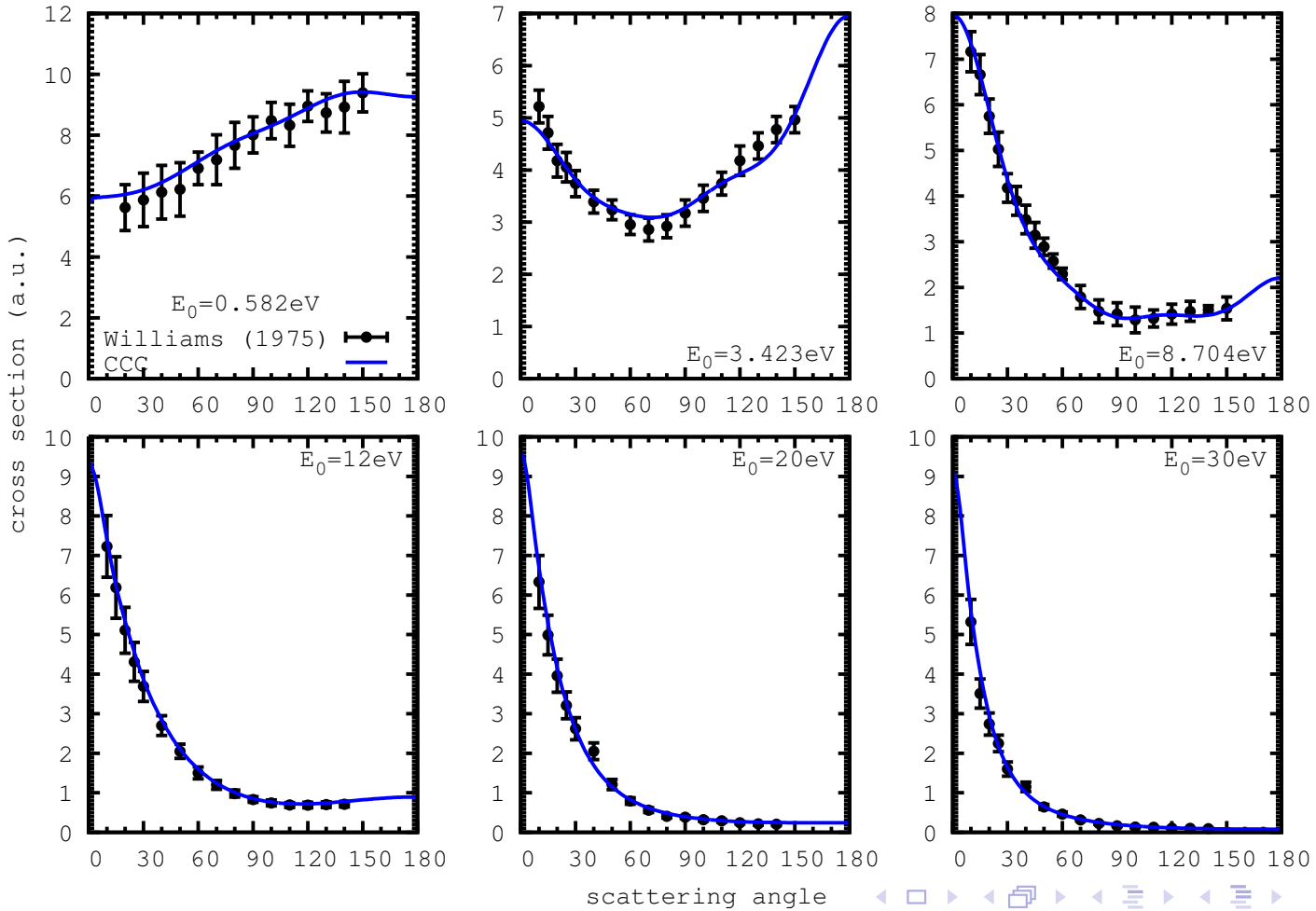
Electron-hydrogen scattering

- total ionization for $n \leq 3$ states



Electron-hydrogen scattering

- elastic differential cross sections



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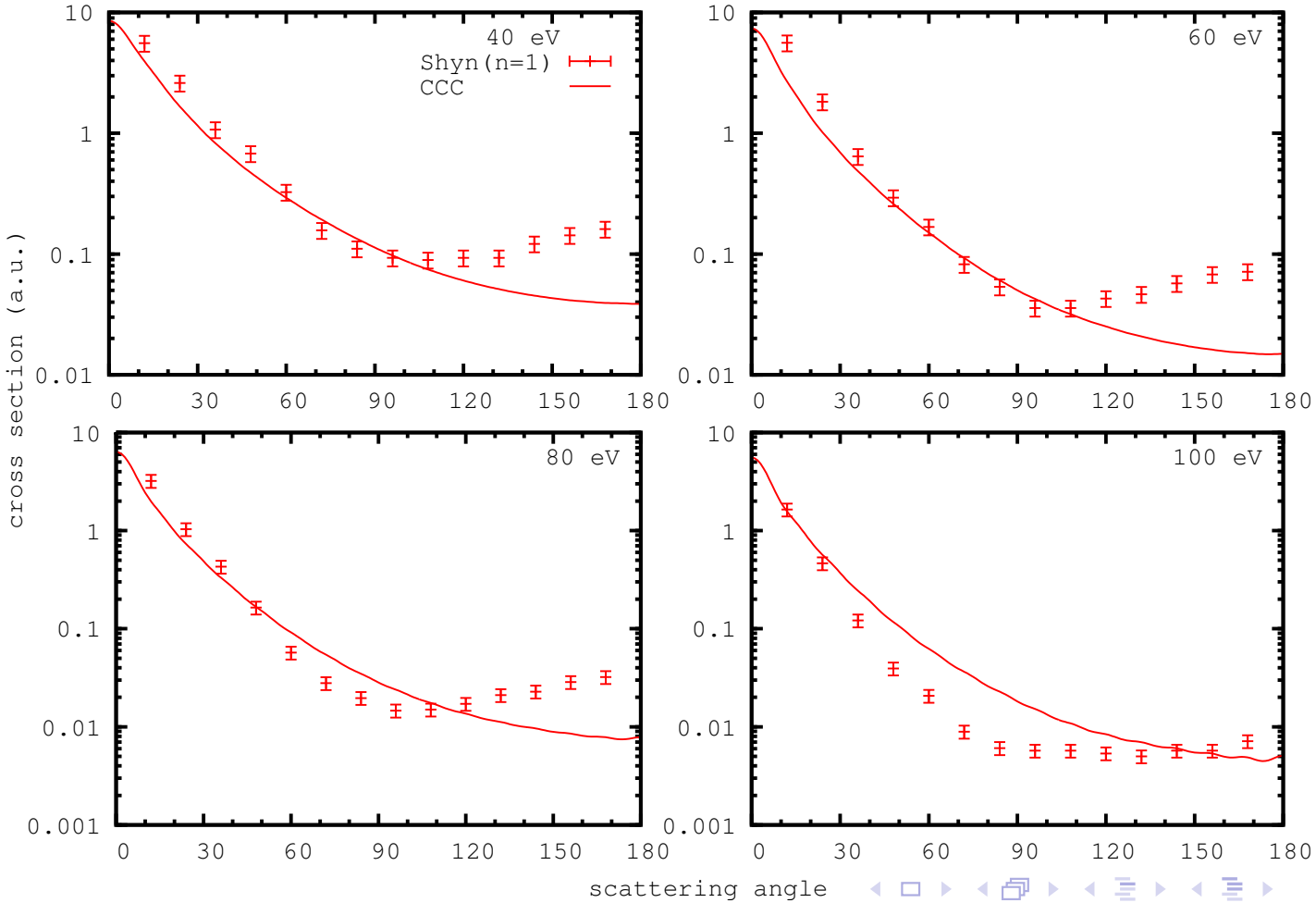
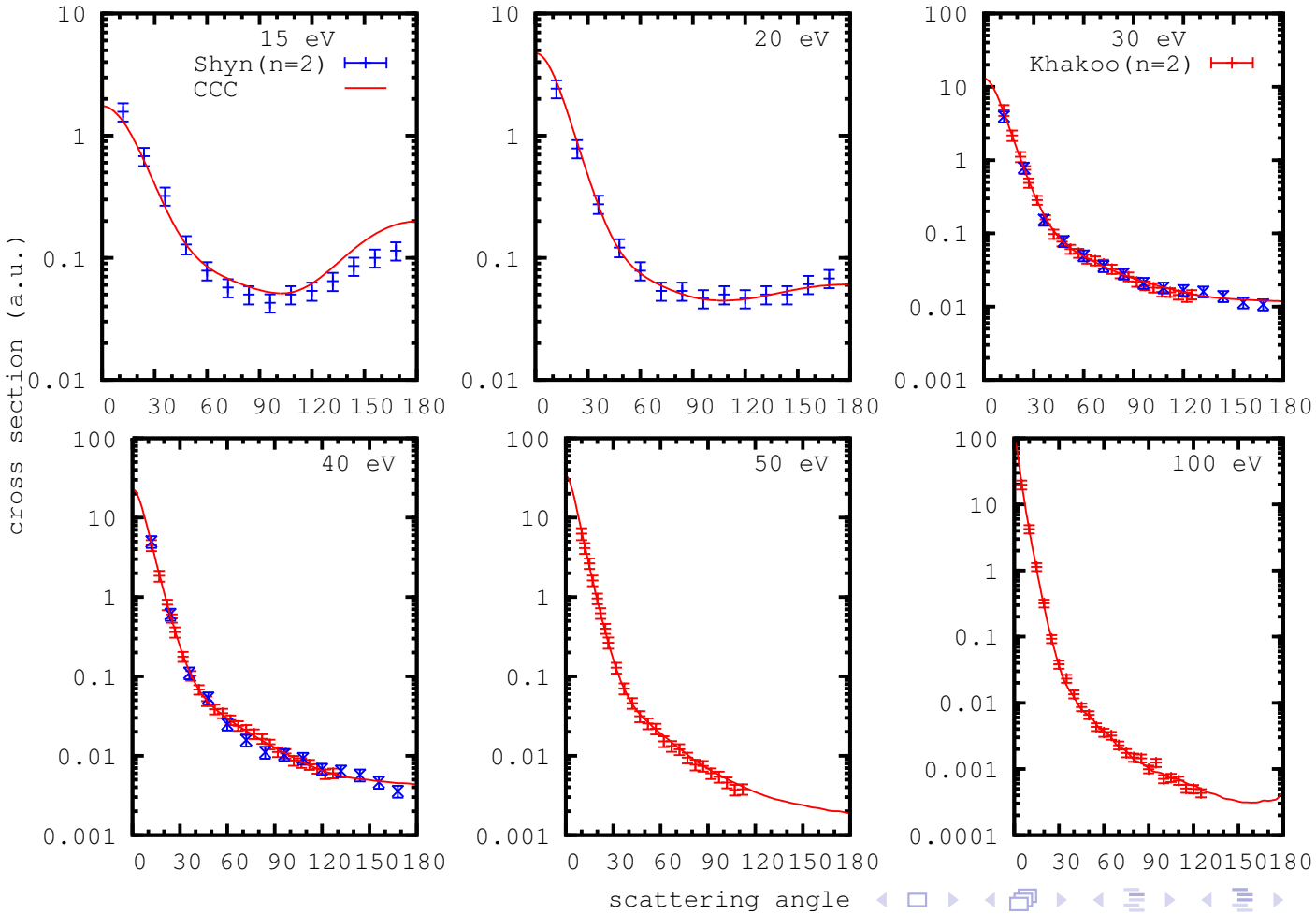


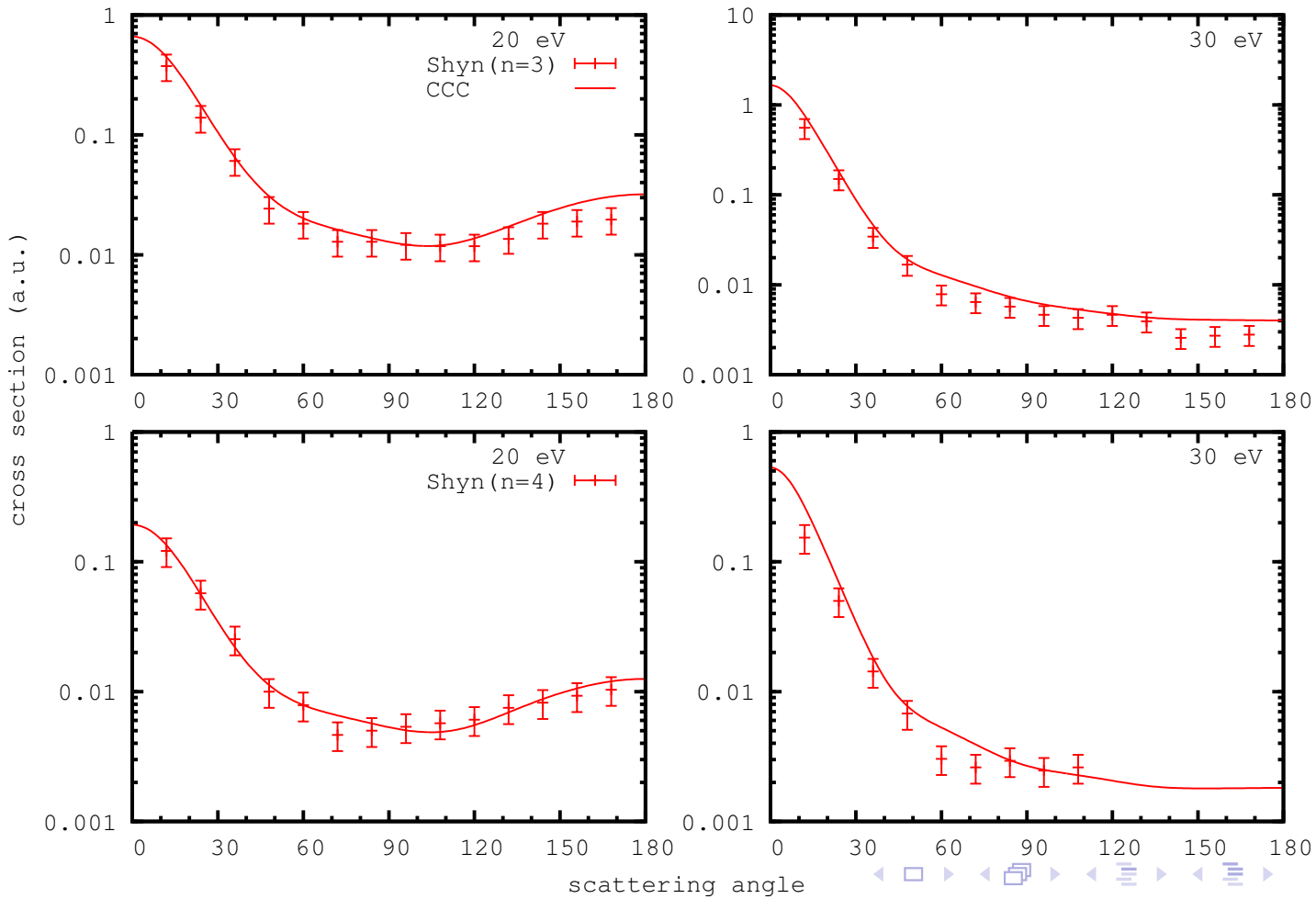
Electron-hydrogen scattering

- $n = 2$ excitation differential cross sections



Electron-hydrogen scattering

- $n = 3, 4$ excitation differential cross sections



Electron-helium scattering

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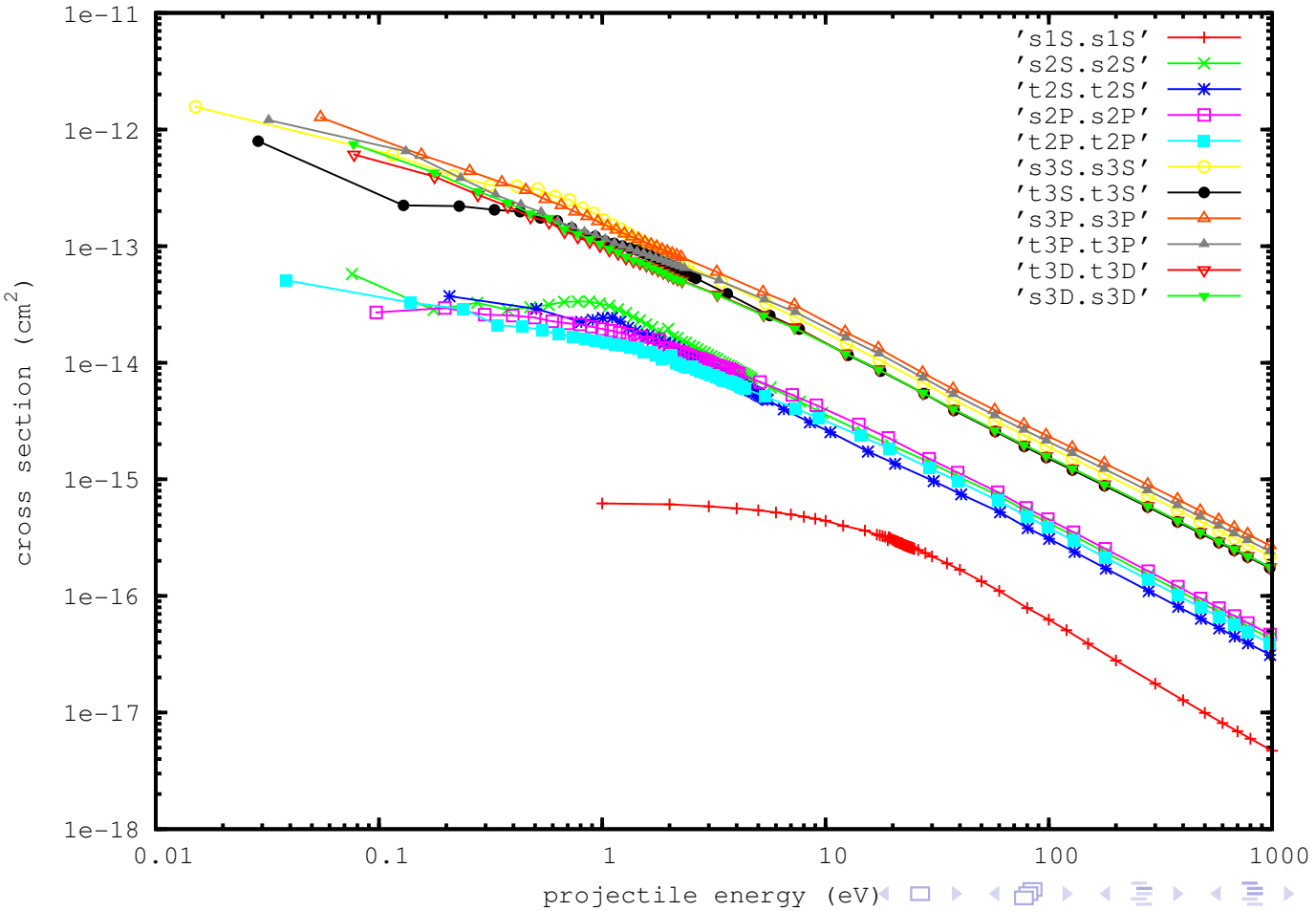

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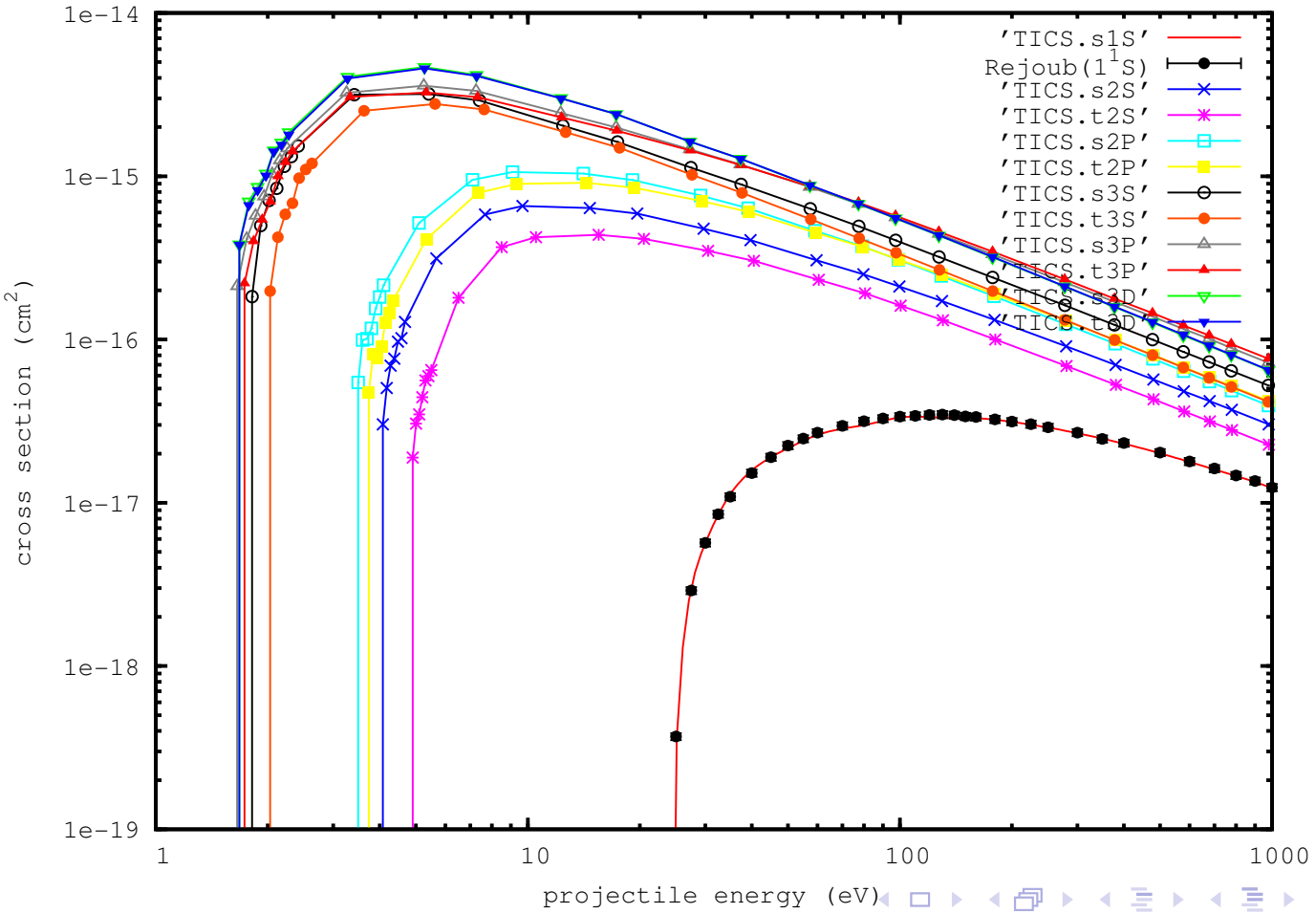

Electron-helium scattering

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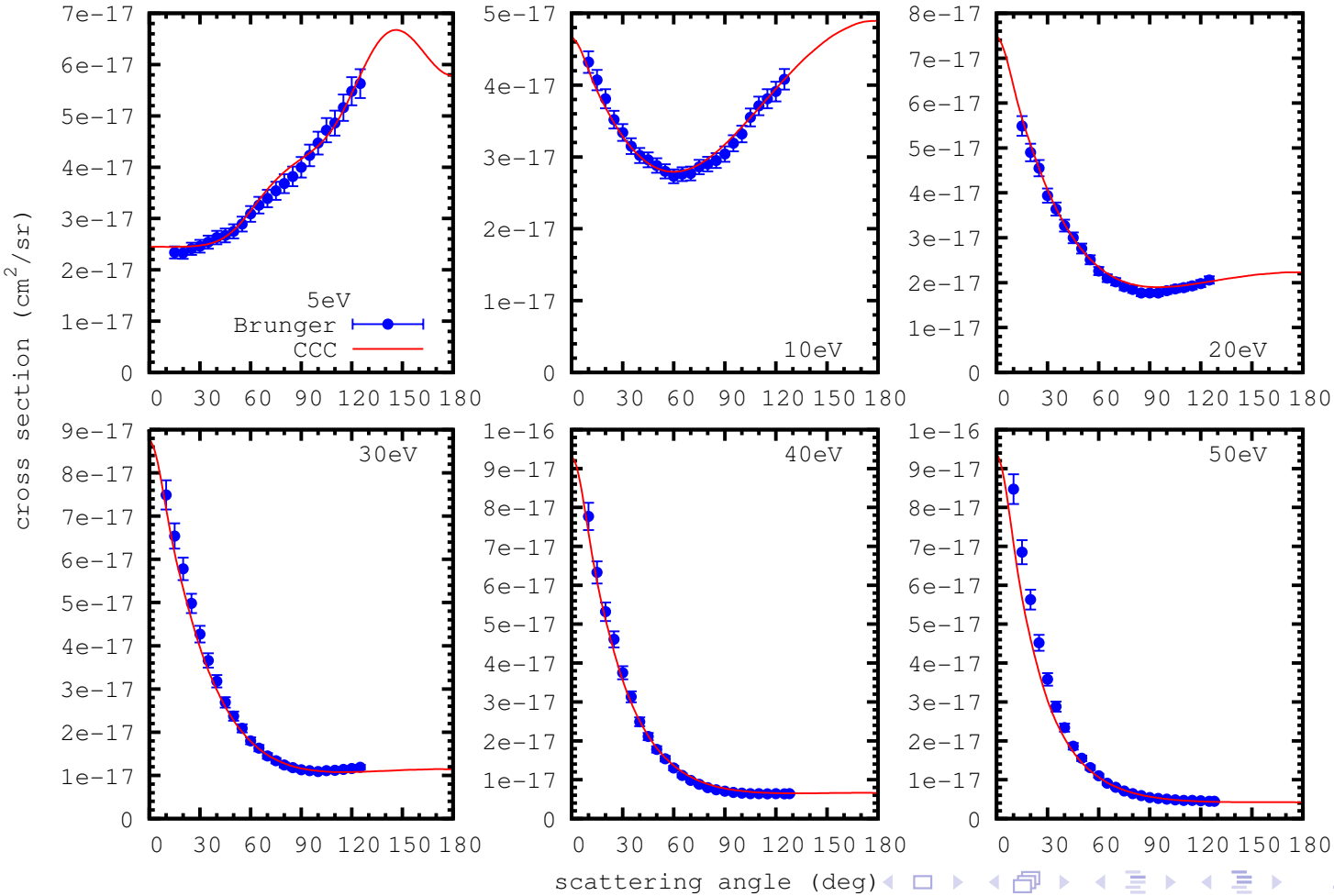
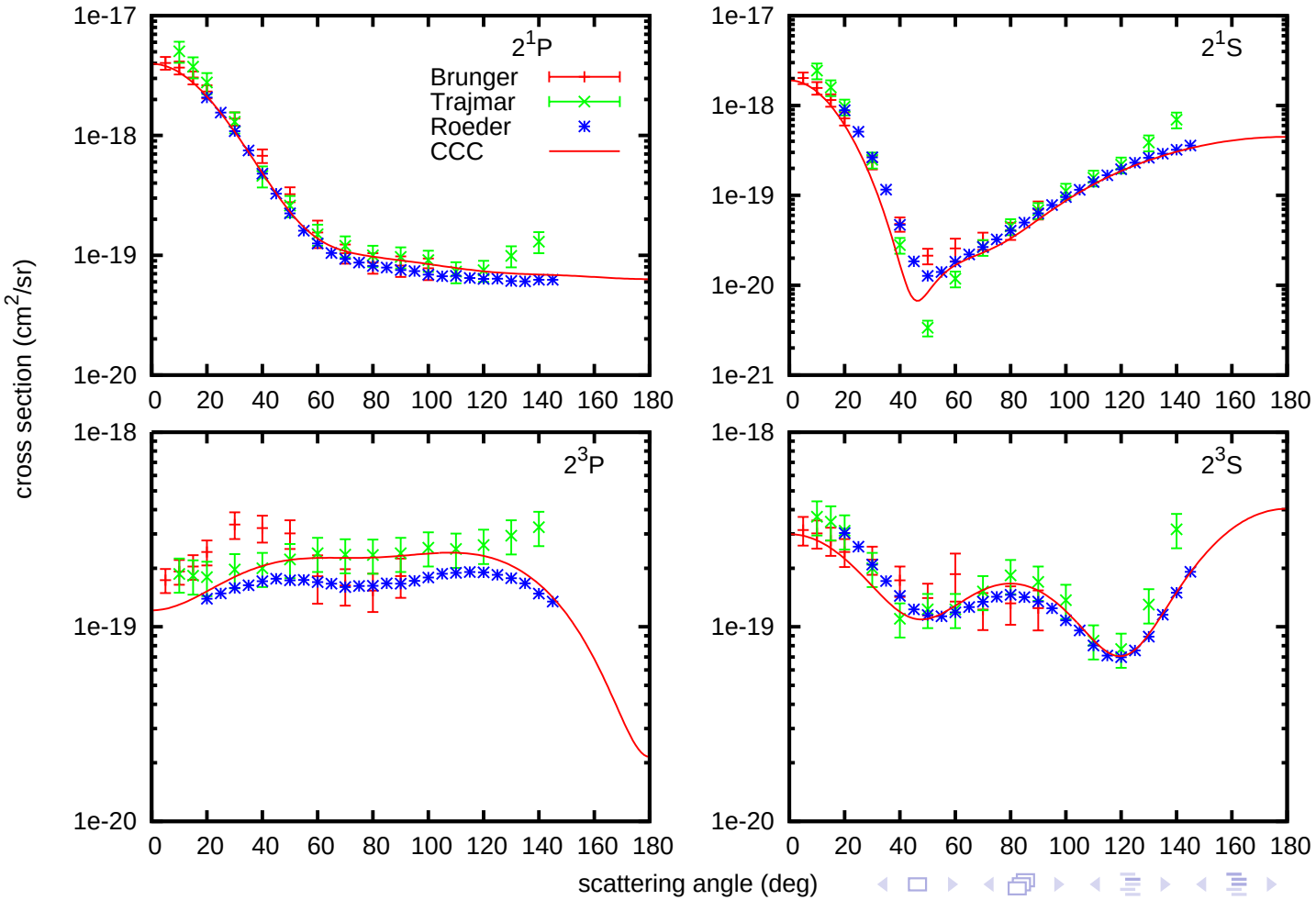


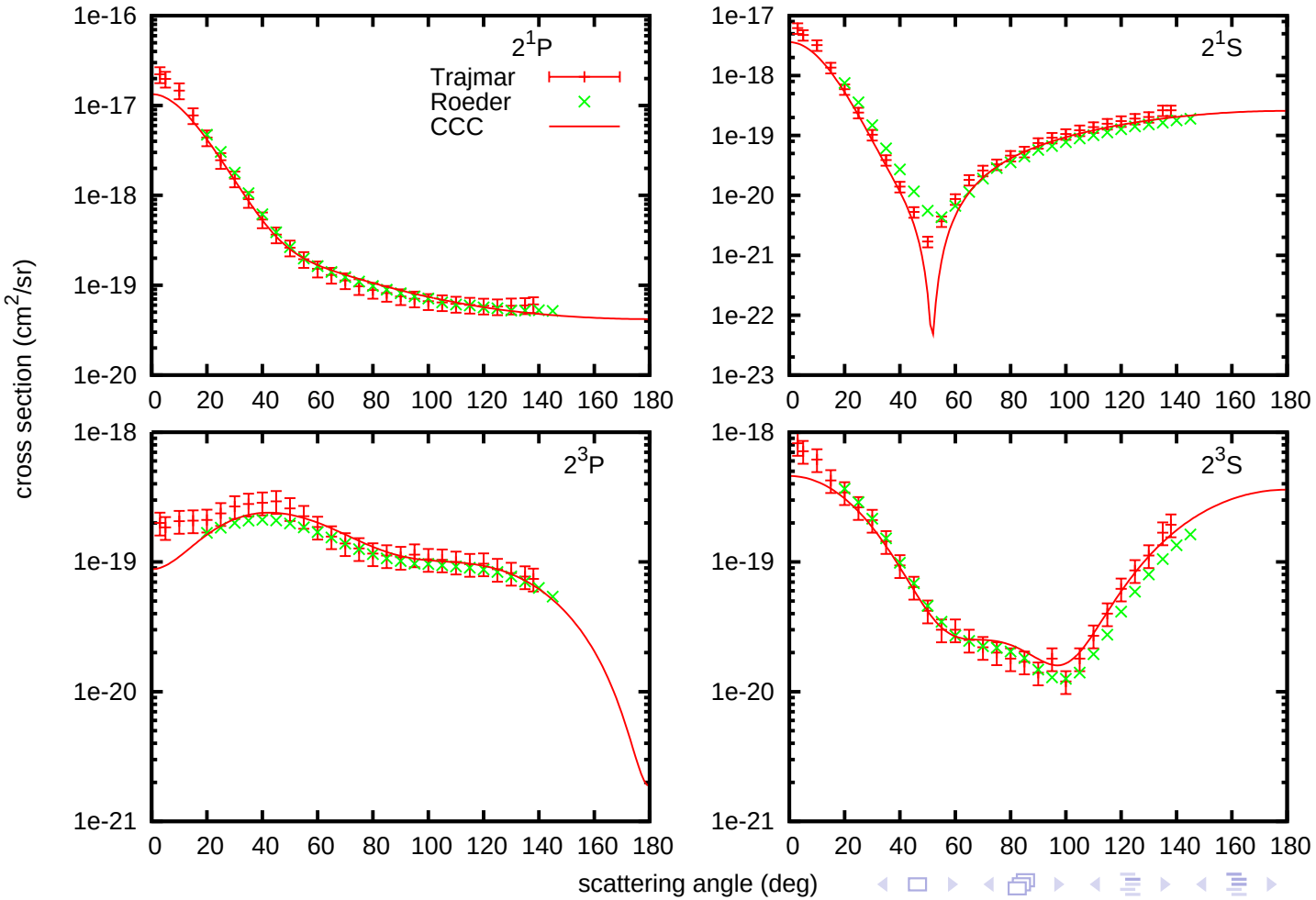
Electron-helium scattering

- 30 eV differential cross sections



Electron-helium scattering

- 40 eV differential cross sections



Concluding remarks

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