Using the R-matrix method to produce accurate data relevant to the plasma community

Electron collisions with H_2 from electronically excited states using the R-matrix method

T. Meltzer[1,2] and J. Tennyson[2]

[1]Institute of Theoretical Physics, Faculty of Mathematics and Physics, Charles University, V Holešovičkách 2, 180 00 Prague 8, Czech Republic
[2]Department of Physics and Astronomy, University College London, London, WC1E 6BT, United Kingdom

1 Introduction

- Electron collisions with H_2 are import for; the semiconductor plasma industry, fusion reactors and astrophysical modeling, amongst others.
- To date, there is a shortage of accurate reference data from both experimental measurements and theoretical calculations.
- We use the R-matrix method as implemented in the UKRMol+ code [1] to compute theoretical cross sections for inelastic collisions of electrons with H_2.

2 Previous Work - Ref. [2]

- We produced benchmark calculations comparing two accurate theoretical methods, R-matrix and Molecular Convergent Close-coupling [3] (MCCC), with experimental and recommended data from literature.
- There was good agreement between the two theoretical methods and recent experimental data, for example see Fig. 1.
- This work focused on excitation from the molecular ground state. This work has been extended to investigate inelastic collisions from initially excited states of H_2.

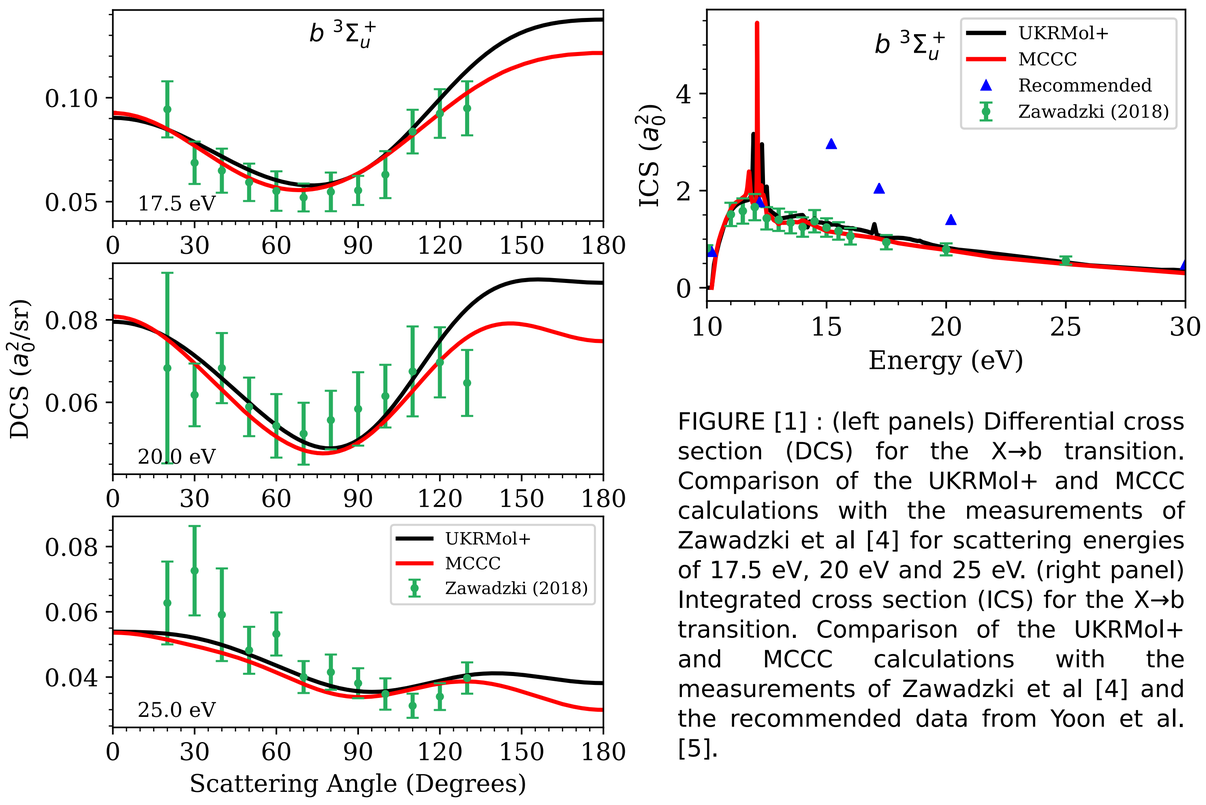

FIGURE [1] : (left panels) Differential cross section (DCS) for the X→b transition. Comparison of the UKRMol+ and MCCC calculations with the measurements of Zawadzki et al [4] for scattering energies of 17.5 eV, 20 eV and 25 eV. (right panel) Integrated cross section (ICS) for the X→b transition. Comparison of the UKRMol+ and MCCC calculations with the measurements of Zawadzki et al [4] and the recommended data from Yoon et al. [5].

3 This Work - Ref. [6]

- Data from initially excited states are almost impossible to obtain experimentally and theoretical data are scarce.
- We extended our previous work to compute 169 separate transitions between the ground and 12 lowest-lying excited states of H_2.
- In Fig. 2 we compare a subset of our calculations with theoretical data available in the literature.

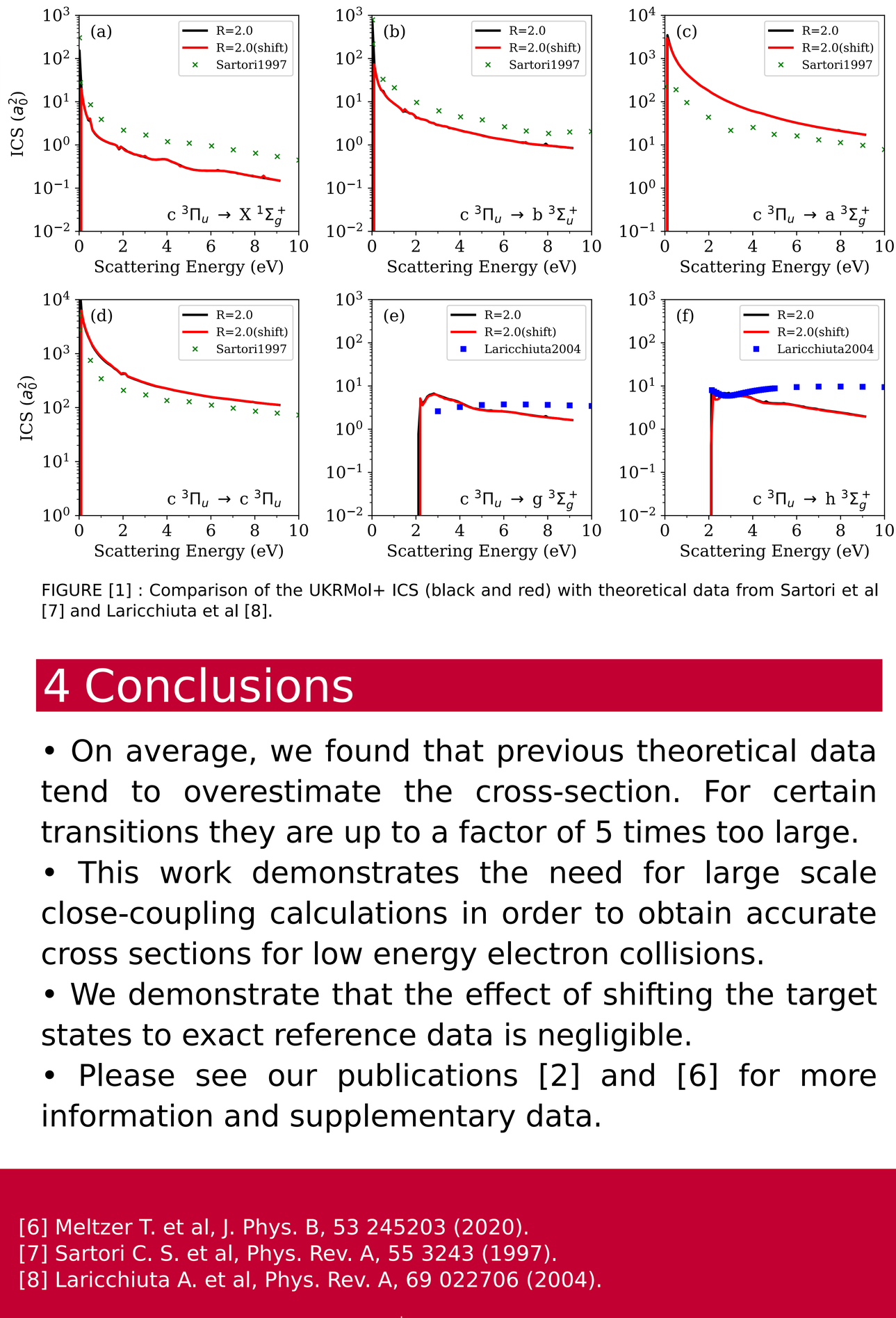

FIGURE [1] : Comparison of the UKRMol+ ICS (black and red) with theoretical data from Sartori et al [7] and Laricchiuta et al [8].

4 Conclusions

- On average, we found that previous theoretical data tend to overestimate the cross-section. For certain transitions they are up to a factor of 5 times too large.
- This work demonstrates the need for large scale close-coupling calculations in order to obtain accurate cross sections for low energy electron collisions.
- We demonstrate that the effect of shifting the target states to exact reference data is negligible.
- Please see our publications [2] and [6] for more information and supplementary data.

References
[1] Mašín Z. et al, CPC, 249 107092 (2020).
[2] Meltzer T. et al, J. Phys. B, 53 145204 (2020).
[3] Zammit M. et al, J. Phys. B, 50 123001, (2017).
[4] Zawadzki M. et al, Phys. Rev. A, 98 062704 (2018).
[5] Yoon J. S. et al, J. Phys. Chem. Ref. Data, 37 913 (2008).
[6] Meltzer T. et al, J. Phys. B, 53 245203 (2020).
[7] Sartori C. S. et al, Phys. Rev. A, 55 3243 (1997).
[8] Laricchiuta A. et al, Phys. Rev. A, 69 022706 (2004).

*thomas.meltzer@utf.mff.cuni.cz