Photoionization cross sections using Quantemol-N

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CORINF Correlated Multielectron Dynamics in Intense Laser Fields

Quantemol

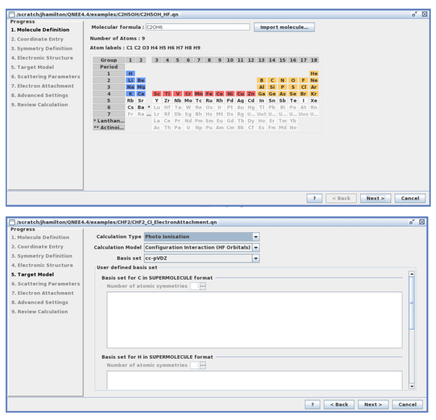
Quantemol Ltd

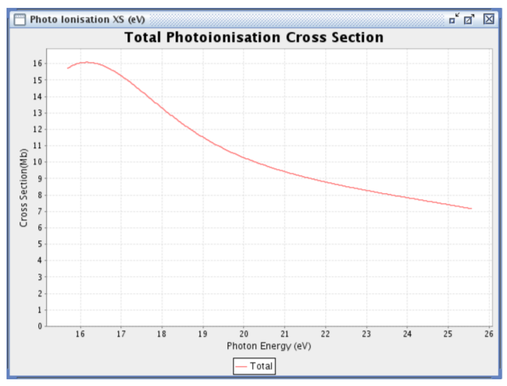
Quantemol is based at University College London and was founded by Prof. Jonathan Tennyson FRS and Dr Daniel Brown in 2004. The company develops unique software tools that bring accessibility to highly sophisticated research codes

QN Electron Scattering

The removal of an electron from an atom or molecule by the action of light, photoionization, is an important process in many environments.

.Models of photoionizing plasmas require accurate cross sections for the species in the plasma. While these are generally available from laboratory experiments for stable molecule, such cross sections are hard to measure for the radicals and ions which provide many of the species that make up a typical molecular plasma.





Quantemol-N is an expert system for performing electron-molecule collision calculations as a function of energy[1]. It provides an easy-to-use interface to the highly-flexible UK Molecular R-matrix codes (UKRMol)[2] . A thorough review of the theoretical methods underlying these codes is available[3]

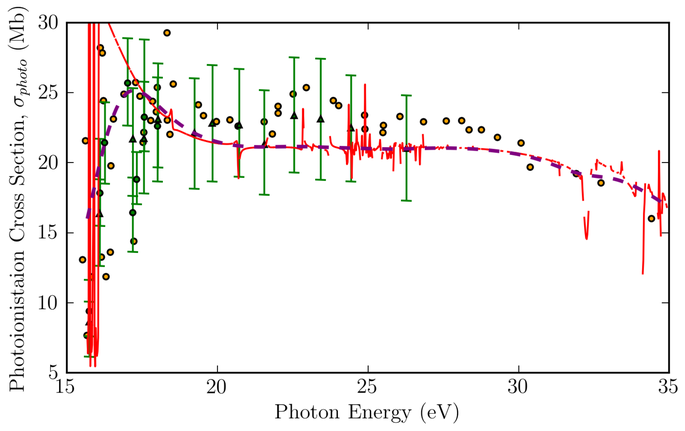
Harvey et al[4] implemented changes to allow the UKRMol codes to perform photoionization calculations. This poster displays some first results from the implementation of this code in Quantemol-N, giving a new photoionisation module.

Calculations

Photon fluxes penetrate deeply into plasmas and affect etching and deposition rates . The code has been tested for a number of molecules. This poster presents results for the photoionization of molecular nitrogen, N_2. Nitrogen is a key component of the Earth's atmosphere and many plasmas for etching and cleaning. There are also good experimental results available for us to make comparisons against.

- Nitrogen target represented with cc-pVTZ basis set
- Target represented with complete active space configuration interaction (CAS-CI) treatment placing the highest 10 electrons in 7 orbitals
- The continuum calculations used a set of s,p,d,g,f symmetry Gaussian orbitals placed at the molecular center-of-mass to represent the photoionized electron
- R-matrix sphere of 12 a_0
- All states up to 30eV generated from the initial CAS-CI calculation included in the final close-coupling expansion
- Calculation converges

Fig. 1 Total photoionization cross-sections for molecular nitrogen: solid and dashed curves, raw and smoothed calculations. Experimental results are: green symbols with error bars are due to Wainfan et *al*[5] and orange bullets are due to Samson *et al*[6].



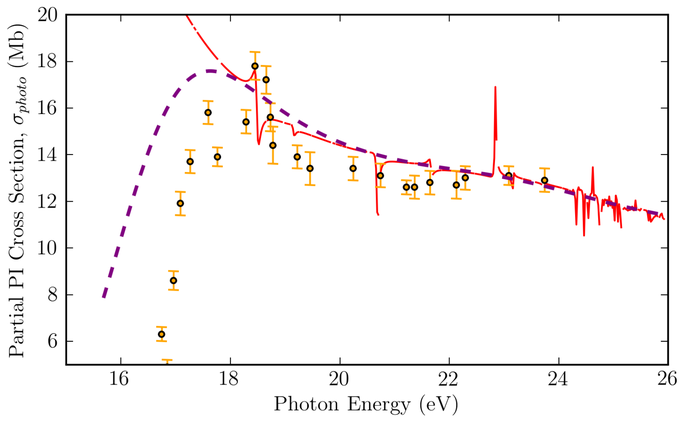


Fig. 3 Partial photoionization cross-sections for molecular nitrogen into the A $^2\Pi_u$ N_2^+ first excited state: solid and dashed curves, raw and smoothed calculations. Experimental results are due to Samson *et al*[6]

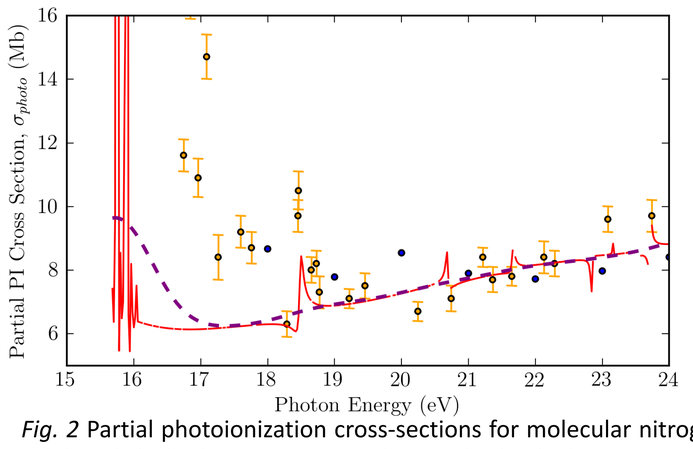


Fig. 2 Partial photoionization cross-sections for molecular nitrogen into the X $^2\Sigma^+_g$ N_2^+ ground stagtes: solid and dashed curves, raw and smoothed calculations. Experimental results are: orange bullets with error bars are due to Samson *et al*[6] and blue bullets are due to Hamnett etl al[7]

- Figure 1 shows Quantemol -N calculations compare well to experimental data and also identifies a number of additional features, known as resonances, particularly at the low energies
- Figures show Gaussian smoothing of calculations to represent how the resonances are washed out in the actual molecule by its vibrational motion
- Figures 2 and 3 show cross-sections for photoionization to the lowest two excited states of the N_2^+ ion, the X $^2\Sigma^+_g$ state and the A $^2\Pi_u$ state, respectively.

Conclusion

We have developed a new easy-to-use and generally applicable code for the calculation of molecular photoionization cross-sections. Further details can be found on the Quantemol website (www.quantemol.com). This code can be used to provide input to plasma modeling codes such as those also provided by Quantemol.

References

1. J. Tennyson, D. B. Brown, J. J. Munro, I. Rozum, H. N. Varambhia and N. Vinci, J. Phys. Conf. Series, **86**, 012001 (2007).
2. J. M. Carr, P. G. Galiatsatos, J. D. Gorfinkiel, A. G. Harvey, M. A. Lysaght, D. Madden, Z. Masin, M. Plummer and J. Tennyson, Euro. J. Phys. D, **66**, 58 (2012).
3. J. Tennyson, Phys. Rep., **491**, 29 (2010).
4. A. G. Harvey, D. S. Brambila, F. Morales and O. Smirnova, arXiv:1401.0229 (2013).
5. N. Wainfan, W. C. Walker and G.L. Weissler, Phys. Rev., **99**, 542 (1955).
6. J. A. R. Samson, G. N. Haddad and J. L. Gardner, J. Phys. B: At. Mol. Opt., 10, 1749 (1977).
7. A. Hamnett and W. Stoll and C.E. Brion, J. Electron Spectrosc., **8**. 367 (1976).

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