Photoionization cross sections using Quantemol-N
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Quantemol Ltd
Quantemol is based at University College London and was founded by Prof. Jonathan Tennyson FRS and Dr Daniel Brown in 2004. Tennyson et al.1 have developed a new easy-to-use code for the calculation of photoionization cross sections for molecular nitrogen into the N2^+ states. This code can be used to provide input to plasma modeling codes such as those also provided by Quantemol.

Calculations
Photon fluxes penetrate deeply into plasmas and affect etching and deposition rates. The code has been tested for a number of molecules. This paper presents results for the photoionization of molecular nitrogen, N2. 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-Cl) treatment placing the highest 10 electrons in 7 orbitals
- The continuum calculations used a set of s,p,d,f symmetry Gaussian orbitals placed at the molecular center-of-mass to represent the photoionized electron
- A matrix sphere of 12 a_0
- All states up to 30 eV generated from the initial CAS-Cl 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 al2 and orange bullets are due to Samson et al.

Fig. 2 Partial photoionization cross-sections for molecular nitrogen into the X^2^+Σ g, N2^+ first excited state; solid and dashed curves, raw and smoothed calculations. Experimental results are: orange bullets with error bars are due to Samson et al2 and blue bullets are due to Hamnett et al2.

Fig. 3 Partial photoionization cross-sections for molecular nitrogen into the X^2^+Σ g, N2^+ ground stages: solid and dashed curves, raw and smoothed calculations. Experimental results are: orange bullets with error bars are due to Samson et al2 and blue bullets are due to Hamnett et al2.

References

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.