Computational studies of few-photon ionisation of molecules irradiated by arbitrarily polarised light

Supervision team: Dr Jimena Gorfinkiel and Dr Sam Eden

Lead contact: Jimena Gorfinkiel

Description: Over the last few years, the development of novel technologies for ultra-short laser pulses and free-electron laser radiation have opened the door to new experiments that are investigating ultra-fast electron dynamics in atoms and molecules [1]. Computational approaches have lagged behind, but recent developments of the UKRmol+ [2] and RMT suites [3] have provided a suite of codes able to treat multielectron dynamics in molecules subject to arbitrarily polarized light. The developed software, based on the R-matrix with time and molecular R-matrix approaches, has so far only been applied to a few simple molecules to study photoionization ignoring the nuclear degrees of freedom [4].

The aim of this project is to exploit this new software tool to study multielectronic effects in few-photon ionization of molecules and its dependence on molecular structure and light polarisation. The project will involve: (i) applying the software in a high-performance computing environment to provide support to novel experiments; (ii) develop an approach to include the nuclear degrees of freedom in the calculations with the aim of modelling the coherent coupled electron and nuclear dynamics.

Opportunities for travel and collaboration will be provided by the Attosecond Chemistry COST Action (https://www.cost.eu/actions/CA18222).

References:

1. K. Ueda et al, J. Phys. B **52** (2019) 171001 (https://doi.org/10.1088/1361-6455/ab26d7)
2. Z. Mašín et al, CPC **249** (2020) 107092 (https://doi.org/10.1016/j.cpc.2019.107092, https://arxiv.org/abs/1908.03018)
3. A. Brown et al, CPC **250** (2020) 107062 (https://doi.org/10.1016/j.cpc.2019.107062, https://arxiv.org/abs/1905.06156)
4. J. Benda et al, PRA **102** (2020) 052826 (https://link.aps.org/doi/10.1103/PhysRevA.102.052826)

Qualifications required:

Applicants must have graduated (or be about to graduate) with an honours degree in Physics, Chemistry or a related discipline and possess good undergraduate-level knowledge of atomic and molecular physics and/or theoretical chemistry. Furthermore, the applicant should have some experience of use of Linux or high-performance computing environments; some software writing experience is also desirable but not essential.