Project title: Probing dipole instabilities in the ultrafast ionization of molecules

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Helpful existing knowledge:	A knowledge of quantum theory and a desire to carry out large-scale calculations on national HPC facilities
Funding status:	Awaiting funding

Project Description:

The energy deposited when molecules interact with radiation sources can initiate a range of electronic and ionic processes in the molecule. These processes can result in the ionization and subsequent fragmentation of the molecule on ultrafast timescales ranging from the attosecond timescale for electronic processes to the femtosecond timescale for fragmentation. These basic interactions lie at the heart of many ultrafast technologies including the design of electronic devices, probes and sensors, biological repair and signalling processes and development of optically-driven ultrafast electronics [1].

Describing these processes on an equal footing is notoriously difficult and several (often quite severe) approximations are usually required. One ab initio method that is widely used to treat the irradiation of molecules is time-dependent density functional theory (TDDFT). In many cases this quantum approach for treating the electron dynamics is coupled to a classical treatment of the ionic dynamics, thus allowing for a non-adiabatic treatment of the electron-ion dynamics. Such an approach is widely used in computational chemistry and materials science for studying the electronic properties of materials. Over the last several years, using our own implementation of TDDFT in an in-house computer package called EDAMAME (Ehrenfest DynAMics on Adaptive MEshes) [2], we have shown that ionization of simple molecules such as nitrogen and acetylene by ultrafast laser pulses results in unexpected dipole instabilities that generate excess electron emission [3, 4]. Understanding the origin of these instabilities is an ongoing area of research involving collaborators in QUB, Toulouse and Erlangen. We have already shown that these instabilities manifest themselves in other theoretical approaches for modelling electron dynamics (such as the Gross-Pitaevskii equation, used for modelling Bose-Einstein condensates). The goal of this project is to understand if these instabilities arise either from the non-linear approaches used for modelling or if they represent a new physical mechanism that can be observed experimentally. Either way, the ramifications of this work are hugely important.

The solution of this problem requires the use of modern high-performance computing technology. The project would therefore suit someone with an interest in both mathematical and computational techniques. A background in maths, physics or physical chemistry would be a distinct advantage. The skills and experience developed during the project are at the leading edge of current technology and will be invaluable in the job market, whether in research or industry.

Useful references

[1] F. Krausz and M. I. Stockman. Nature Photonics **8** 205 (2014)

[2] D. Dundas. J Chem Phys **136** 194303 (2012)

[3] P.-G. Reinhard, et al. Phys Rev A **107** L020801 (2023)

[4] D. Hughes et al. Euro Phys J D **77** 177 (2023)