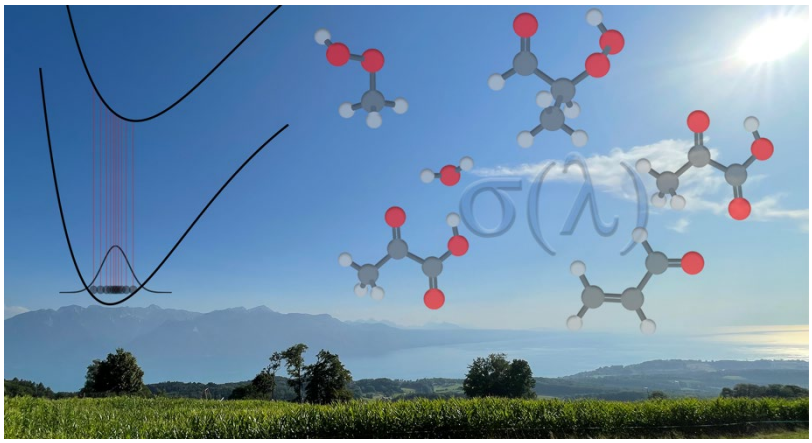
Calculating photoabsorption cross-sections for atmospheric volatile organic compounds

About the project or challenge area: Understanding the chemical and photochemical reactions taking place in the atmosphere is paramount to predicting its composition. A large number of the atmospheric volatile organic compounds (VOCs) are transient species, presenting a real challenge for experimentalists to characterise them. Computational chemistry is often used to provide missing experimental data to the models used to simulate the atmosphere composition. While ground state properties of molecules are rather simple to compute, obtaining information about their excited electronic states constitutes a real challenge. Key analysis of experimental data would nevertheless require properties of molecules such as absorption spectra (or photoabsorption cross-sections), or information about the reactivity of a VOC following light absorption. In this project, you will learn how to use advanced computational techniques aiming at calculating photoabsorption cross-sections and simulating the excited-state dynamics of a molecule.



Why choose this opportunity? The focus of your project will be on theoretical and computational chemistry, which will provide an excellent platform to learn about the properties of molecules. Your work in this area can make a real impact on global challenges, such as the influence of photochemical reactions for the removal of transient VOCs in the atmosphere and their contribution to the formation of secondary pollutants. You will develop and increase your expertise in computational chemistry and using quantum-chemical packages, whilst becoming familiar with the fundamentals of the interaction between light and molecules. Furthermore, this project will require your collaboration with other members across other research groups, thus improving your teamwork and networking skills. You will also develop a range of transferable skills, including presentation, scientific writing, and project and time management. Finally, you will be interacting with students from all over the world learning from their culture and skills, adding to your professional and personal development.

Full training will be provided for all aspects of this project. You will be embedded in the Supervisor's research group, who will provide support. In addition, you will be assigned a mentor for the duration of your project, who will provide extra support and help you to identify any additional training needs or opportunities.

About you: Ideally you will already have skills and knowledge in basic computational chemistry and the use of Linux, teamwork and time management.

Bench fees: A bench fee of £3000 is required.

How to apply: Applications are accepted throughout the Academic Year, and you should complete the online application form for Chemistry (MSc by Research).

Supervisor: Your supervisor for this project will be Basile Curchod, Associate Professor in the School of Chemistry. You can contact him by email basile.curchod@bristol.ac.uk.

Find out more about your prospective research program: This recent work from our group provides some general background on calculating photoabsorption cross-section for atmospheric molecules:

Calculating Photoabsorption Cross-Sections for Atmospheric Volatile Organic Compounds
ACS Earth Space Chem., 2022, 6, 207–217 https://pubs.acs.org/doi/10.1021/acsearthspacechem.1c00355