Project 3.10 Computational Modelling of Cross-Beam Radiation-Matter Interactions

Supervisor: dr hab. Adam Kubas / dr Dariusz Piekarski
Institut: Physical Chemistry
Unit: Research group No. 20 Cooperative catalysis - dr hab. Adam Kubas (contact to: dpiekarski[at]ichf.edu.pl)
www: http://coopcat.pl/

Background:

This computational project aims to investigate theoretically the evolution of various molecular targets including chiral molecules and molecular clusters of 1,2,3-triazole derivatives induced by femto- and nanosecond laser pulses including the effects of chiral light. The main objective is to predict the experimental conditions (excitation energy, charge state, and/or low-lying excited states) for a controlled evolution of the triazole derivatives that can lead to de-click reaction. Molecular dynamics and potential energy surface studies will provide several possibilities to probe the theoretical conditions needed to obtain the aforementioned fragmentation pattern. We will take into account the chemical nature of the triazole derivatives (different substituents, including the chiral centers) as well as the environmental effects by aggregating them into clusters.

The successful candidate will use and further examine the broad spectrum of electronic structure methods. Both the electronic and nuclear stopping power effects will be taken into account theoretically. Possibility to implement quantum methodologies such as nudge elastic band method into Automekin program for electronically excited states will be available. The theoretical work will be supported by our homemade cross-beam light-matter experiments as well as by the collaborative work with our colleagues from leading European cross-beam experimental centers: CNRS (France), CNR, (Italy) ELI (Czech Republic). Prospective candidates are required to possess an MSc degree in Physics, Chemistry, Mathematics, Computational Science, or a closely associated field at the commencement of the studentship. Additionally, a profound inclination towards theoretical and computational methodologies within the realm of atomic, molecular, and optical physics is expected. The financial support encompassed in this opportunity comprises a stipend exempt from taxation, provisions for conference travel, consumables, and coverage of tuition fees for those meeting the criteria for fee eligibility at our Institute of Physical Chemistry, Polish Academy of Sciences.

If you have any informal inquiries regarding the project, the research team, or the application process, please feel free to reach out to PI Dr Dariusz G. Piekarski at dpiekarski(at)ichf.edu.pl

Aim:

The main objective is to predict the experimental conditions (excitation energy, charge state, and/or low-lying excited states) for a controlled evolution of the triazole derivatives that can lead to de-click reaction. Molecular dynamics and potential energy surface studies will provide several possibilities to probe the theoretical conditions needed to obtain the aforementioned fragmentation pattern. We will take into account the chemical nature of the triazole derivatives (different substituents, including the chiral centers) as well as the environmental effects by aggregating them into clusters.

Requirements:

- Prospective candidates are required to possess an MSc degree in Physics, Chemistry, Mathematics, Computational Science, or a closely associated field at the commencement of the studentship,

- additionally, a profound inclination towards theoretical and computational methodologies within the realm of atomic, molecular, and optical physics is expected,
- the financial support encompassed in this opportunity comprises a stipend exempt from taxation, provisions for conference travel, consumables, and coverage of tuition fees for those meeting the criteria for fee eligibility at our Institute of Physical Chemistry, Polish Academy of Sciences.