Contribution ID: **67** Type: **On-site planned, but remote also possible**

Ultrafast relaxation and fragmentation dynamics of astrochemically-relevant molecules investigated by pump-probe experiments at Free-Electron Lasers

Polycyclic aromatic hydrocarbons (PAHs) are a set of molecules consisting of multiple fused aromatic rings. They are especially interesting in the context of the complex chemistry occurring in the interstellar medium (ISM). The first few (substituted) PAHs, indene, 1-cyanonaphthalene, and 2-cyanonaphthalene have been detected in the ISM [1,2,3], and many more are thought to exist because of characteristic infrared emission signatures of PAHs measured as Unidentified Infrared Bands [4]. PAHs are particularly relevant for studies involving FELs since the extreme conditions in the ISM can be mimicked in a laboratory set-up and studied using intense XUV and X-ray radiation, also known to be ubiquitous in the ISM. With such experiments we can delve deeper into the photophysical and photochemical processes that are thought to occur in the ISM. To study the various chemical processes which occur under such conditions, such as ionisation, fragmentation, and isomerisation, we use ultrashort pulses provided by intense free-electron lasers (FELs). This is because such processes happen on very short timescales (~femtoseconds) [5,6] and FELs provide unprecedented opportunities to explore such processes.

The measurements for the ultrafast pump-probe experiments of PAHs have already been performed at Free-electron LASer at Hamburg, FLASH, where time-of-flight mass spectrometry (TOF-MS) and velocity-map imaging (VMI) techniques were employed. Apart from analysis of this TOF-MS and VMI data, a well known covariance analysis method [7] can also be applied to get a deeper insight into the reactions occurring at these timescales.

This project focuses on handling the complex data acquired during these experiments while also learning the analysis tools for the same. Handling the data, which is in h5 or binary file format, will involve usage and development of the libraries using Python programming language. To gain a deeper understanding of the experimental data, it can also be corroborated with theory using quantum chemical calculations. Further, an interpretation of the results would lead to an understanding of the fragmentation patterns and dynamics of the astrochemical relevant PAHs through a combination of TOF-MS, VMI, and covariance analysis. Overall, the project would be composed of around 40% of time spent in learning and applying the software, and 60% of time spent in analysing the results using physics and chemistry principles. The investigation of PAHs using these techniques will append our knowledge of the complex femtochemistry occurring in the ISM.

References:

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[4] Peeters, E., et al. "The rich 6 to 9 m spectrum of interstellar PAHs." Astronomy & Astrophysics 390.3 (2002): 1089-1113.

[5] Lee, J. W. L., et al. "Time-resolved relaxation and fragmentation of polycyclic aromatic hydrocarbons investigated in the ultrafast XUV-IR regime." Nature Communications 12.1 (2021): 1-11.

[6] Marciniak, Alexandre, et al. "XUV excitation followed by ultrafast non-adiabatic relaxation in PAH molecules as a femto-astrochemistry experiment." Nature Communications 6.1 (2015): 1-6.

[7] Frasinski, Leszek J. "Covariance mapping techniques." Journal of Physics B: Atomic, Molecular and Optical Physics 49.15 (2016): 152004.

Field

A2: Molecular sciences (application oriented)

DESY Place

Hamburg

DESY Division

FS

DESY Group

FS-SMP

Special Qualifications:

Elementary knowledge in Python programming would be beneficial.

Primary authors: GARG, Diksha (FS-SMP (Spectroscopy of molecular processes)); SCHNELL, Melanie (DESY); CHOPRA, Pragya (FS-SMP (Spectroscopy of molecular processes))