A call for a 3-year PhD is open in Barcelona.

Would yo like to do a PhD in computational physics/chemistry/biochemistry?

Do you like the idea of healing diseases with X-ray lasers?

The date of incorporation is between September 2021 and March 2022. We need to apply for a grant from the Catalan Government. The deadline to apply for the grant is 15 March 2021.

All the documentation to apply for the grant has to be prepared before that date, so that someone interested should **contact me before Tuesday 9 March** (carles.serrat-jurado@upc.edu)

The candidate will work in the frame of the project:

"Perspectives for hard X-ray selective cancellation of the effect of target molecules in pathogens",

as described in the WavemiX 2021 Book of
Projects https://indico.psi.ch/event/10556/page/1961-about-wavemix

Abstract:

We have recently studied four-wave mixing processes with FELs pulses around the atomic edges exploiting the random phase characteristics of ω-3ω pulses and concluded that the anti-Stokes 5ω component can be efficiently generated with high spectral selectivity. In this project, we propose to explore the low-dose regime, using hard X-rays as in medical imaging, to selectively cancel the effect of the active center of specific molecules maybe combined with molecule labellings in pathogens such as viruses, bacteria or cancer cells, and hence also to establish an innovative technique in the cure of diseases such as Alzheimer's.

Short description:

X-ray absorption spectroscopy may provide a unique absorption spectrum that can serve as a fingerprint of the state of a particular atom or molecule. It was reported that exposure to laser-produced X-rays pulses with relatively high peak intensities does not lead to increased harm to mammalian cells exposed in vitro compared with the harm induced from exposure to X-rays with the same dose from conventional medical sources, concluding that the use of high-power laser facilities for medical imaging is justified [1]. We propose to study both through numerical simulations and experimentally the capability of the four-wave mixing (FWM) effect described in [2] at relatively low laser peak pulse intensities in biomolecules maybe also combined with biomolecules labellings. Initially the optimal biomolecules targets and possible labeled molecules have to be identified by characterizing with precision their X-ray absorption spectra. As first tests, we will consider simple zinc complexes that have recently been characterized [3], to later study more realistic metalloproteins active centers and other molecules. We hence expect to be able to effectively produce nonlinear FWM processes

locally and selectively in some biologically relevant molecules using ultrashort laser pulses with medical harmless doses (mGy).

[1] C. Tillman et al., "Survival of Mammalian Cells Exposed to Ultrahigh Dose Rates from a Laser-produced Plasma X-ray Source", Radiology 1999, 213, 860–865.
[2] C. Serrat, "Localized Core Four-Wave Mixing Buildup in the X-ray Spectrum of Chemical Species", J. Phys. Chem. Lett. 2021, 12, 1093−1097.
[3] O. M. Stepanic et al., "Probing a silent metal: A Combined X-ray Absorption and Emission Spectroscopic Study of Biologically Relevant Zinc Complexes", Inorg. Chem. 2020, 59, 13551−13560.