"PHOTOCHEMISTRY AND SPECTROSCOPY WITH MULTIREFERENCE PERTURBATION THEORY"

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February 26, 2021 (Friday)
12pm (BRT time) - Google Meet

ORGANIZATION:
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INFORMATION AND REGISTRATION:
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with the words "Javier Segarra-Martí– Virtual" on the "subject"
Deadline: February 24, 2021 (Wednesday), 06pm (BRT time)

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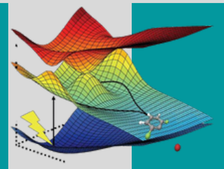

ABSTRACT

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The field of molecular excited state simulations have witnessed a renewed interest as it leverages essential processes in biological and nanotechnological applications, such as DNA damage or artificial light harvesting. Initially rooted on the computation of potential energy surfaces of simple molecules in gas phase and a stick representation of spectral fingerprints, theoretical photochemistry has now evolved to time-resolved non-adiabatic dynamics studies and the characterisation of spectral lineshapes from first principles.[1]
In this seminar I will briefly describe some of the tools developed to connect theory with experiment in the simulation of realistic environments and non-linear optical spectroscopies.[2,3] I will focus mostly on work carried out recently to characterise the photophysical
properties of DNA/RNA nucleobases and nucleosides, which will be covered from static, dynamic and spectroscopic standpoints,[4] as well as considering both UV (photo-excitation)[5-8] and VUV (photo-ionisation) [9,10] triggered events.

[1] I. Conti et al., J. Am. Chem. Soc. 2020, 142, 16117–16139.
[2] J. Segarra-Martí et al., Top. Curr. Chem. 2018, 376, 24–72.
[3] O. Weingart et al., J. Mol. Model. 2018, 24, 1–30.
[4] J. Segarra-Martí et al., Faraday Discuss. 2020, 221, 219–244.
[5] A. J. Pepino et al., J. Phys. Chem. Lett. 2017, 8, 1777–1783.
[6] L. Martínez-Fernández et al., J. Am. Chem. Soc. 2017, 139, 7780–7791.
[7] A. J. Pepino et al., Phys. Chem. Chem. Phys. 2018, 20, 6877–6890.
[8] J. Segarra-Martí et al., In preparation.
[9] J. Segarra-Martí et al., Phys. Chem. Chem. Phys. 2019, 21, 14322–14330.
[10] J. Segarra-Martí et al., ChemPhotoChem 2019, 3, 856–865.