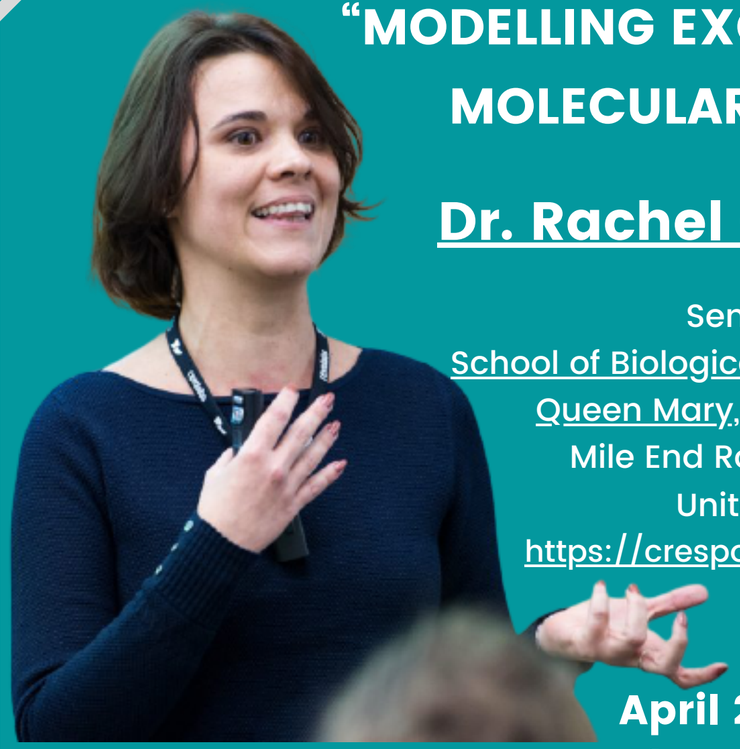
"MODELLING EXCITED STATES IN MOLECULAR CRYSTALS"



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April 23, 2021 (Friday)
12pm (BRT time) - Google Meet

ORGANIZATION:
Prof. Dr. Antonio Carlos Borin
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INFORMATION AND REGISTRATION:
ancborin@iq.usp.br

Registration: send a message to ancborin@iq.usp.br
with the words "Rachel Crespo-Otero - Virtual" on the "subject"
Deadline: April 21, 2021 (Wednesday), 06pm (BRT time)

WEBINARS COMPUTATIONAL PHOTOCHEMISTRY

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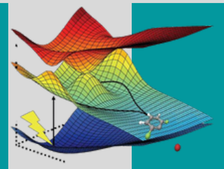

ABSTRACT
Modelling excited states in molecular crystals

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Light-emitting materials find applications in display technologies, optical communication, data storage, biological sensing and solid-state lasing. Aggregation-induced emission (AIE) offers a route for the development of luminescent technologies with high quantum efficiencies. However, maximising fluorescence quantum efficiencies is a formidable challenge in attaining first-principles materials design, due to the interplay between the electronic structure of the chromophore and the molecular crystal. The identification of radiative and nonradiative channels, and how these are affected by aggregation, can help rationalise the emissive properties of materials and aid in the design of yet more efficient fluorophores.

In this talk, I will discuss how inter- and intramolecular processes determine the emissive properties of a series of crystals including prototypical propeller-shaped AIE, intramolecular proton transfer chromophores and aromatic molecules with applications in lasers (1–4). The excited state mechanisms will be examined considering the competition between nonradiative and radiative pathways. The role of conical intersections will be addressed in the context of the 3D-structure of the crystals, exciton couplings and the presence of triplet states. The fromage (FRamewOrk for Molecular AGgregate Excitations) platform (5,6) will be presented as a tool to assist with the investigation of photochemical processes in molecular crystals.

References:
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