

# Webinars on Computational Photochemistry

## "CASPT2 Determinations of Molar Extinction Coefficients in Condensed Phases"

[Dr. Daniel Roca-Sanjuán](#)

Quantum Chemistry for the Excited State (QCEXVAL)

[Institute of Molecular Science \(ICMol\)](#), University of Valencia, Spain

December 11, 2020 (Friday) **02:30pm (BRT time)**

Google Meet

Organization: [Prof. Dr. Antonio Carlos Borin](#)

[Instituto de Química, Universidade de São Paulo \(USP\), SP, Brazil](#)

Information and Registration: [ancborin@iq.usp.br](mailto:ancborin@iq.usp.br)

Registration: send a message to [ancborin@iq.usp.br](mailto:ancborin@iq.usp.br)

With the words "Daniel Roca-Sanjuán – Virtual" on the "subject"

Deadline: December 09, 2020 (Wednesday), 06pm (BRT time).



# CASPT2 Determinations of Molar Extinction Coefficients in Condensed Phases

[Dr. Daniel Roca-Sanjuán](#)<sup>1</sup>, Ana Borrego-Sánchez<sup>2</sup>

<sup>1</sup>[Institut de Ciència Molecular](#), Universitat de València, València, Spain

<sup>2</sup>[Instituto Andaluz de Ciencias de la Tierra](#) (CSIC-University of Granada), Granada, Spain

In materials and biological systems, chromophores are confined to distinct types of chemical and physical environments, for instance, water solution, inside a pore, at the interlayer space of layered materials, etc. Spectroscopic properties derived from the interaction between the chromophores and light might be affected by the environment giving rise to changes with respect to the behavior of the isolated system. By using computational chemistry, a semiquantitative description of the physicochemical effects of light-matter interaction can be already obtained by studies with the isolated molecule. Nevertheless, to improve such description and provide a more realistic description, the environment must be considered.

In this work, we shall focus on the determination of molar extinction coefficients, ( $\epsilon$ ) of chromophores in condensed phases and in a wide range of wavelengths. For an accurate prediction of  $\epsilon$ , two requirements are needed: (i) an accurate methodology for describing correctly both the ground and the distinct types of excited electronic states and (ii) a computational approach to sample the conformational space of the chromophore-environment complex. Regarding the first point, multiconfigurational quantum chemistry (mainly based on the complete-active-space second-order perturbation theory (CASPT2) method) with the OpenMOLCAS software is a practical option, specially competitive (as compared to others) for electronic transitions to high-energy excited states with important contributions of multiply-excited configuration state functions. For the conformational sampling, distinct approaches are available, such as molecular (classical) dynamics, semiclassical dynamics or Wigner sampling, among others. We shall compare in this contribution the performance of the three mentioned sampling strategies used with the CASPT2 method and combining the programs OpenMOLCAS and Materials Studio (or AMBER) to determine the  $\epsilon$  of chromophores in solution and at the water – gas phase interface. Even though the approach does not provide the user with the rovibrational resolution of the bands, the absorption line shapes can be determined obtaining a good agreement with the experimental data.