"ATTOCHEMISTRY: CONTROLLING THE ELECTRONS IN EXCITED STATE CHEMISTRY"

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October 08, 2021 (Friday)
12pm (BRT time) - Google Meet

ORGANIZATION:
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INFORMATION AND REGISTRATION:
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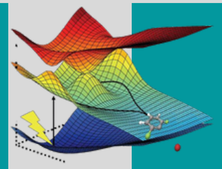
Registration: send a message to ancborin@iq.usp.br
with the words "Michael Robb – Virtual" on the "subject"
Deadline: October 07, 2021 (Thursday), 06pm (BRT time)



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ABSTRACT

Attochemistry: Controlling the Electrons in Excited State Chemistry

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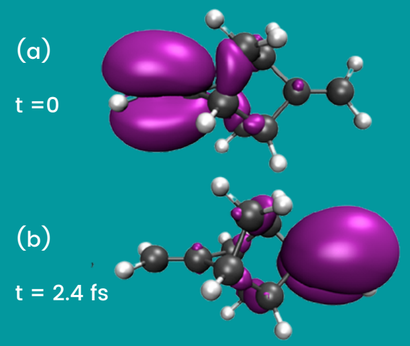
Light pulses, of attosecond (1 as = 10^{-18} s) duration, can populate several electronic states coherently. This has opened up the possibility of observing electron dynamics driving (controlling) the nuclear dynamics. We have been studying such electron dynamics together with the coupled nuclear motion, using our implementation of the Ehrenfest method (for electronic wavepackets) with quantized nuclear motion (Quantum Ehrenfest QuEh method) (1). The initial electronic wavepacket is chosen as a superposition of excited states. If this superposition is chosen appropriately, it can be used to steer the coupled nuclear motion, and thus leads to attochemistry.

We will review our methodology (1) for the combination of the Ehrenfest method with both classical and quantum dynamics (2). We will then focus on some model (3, 4) molecular systems where the course of the nuclear motion is driven by the nature of the electron dynamics.



1. A. Jenkins, K. Spinlove, M. Vacher, G. Worth and M. Robb, Journal of Chemical Physics 149 (2018).
2. K. G. G. A. Worth, G. W. Richings, I. Burghardt, M. H. Beck, A. Jäckle, and H.-D. Meyer. The QUANTICS Package, Version 1.1, (2015), University of Birmingham, Birmingham, U.K., (2015).
3. T. Tran, G. A. Worth and M. A. Robb, Communications Chemistry 4 (1), 48 (2021).
4. M. Olivucci, T. Tran, G. A. Worth and M. A. Robb, The Journal of Physical Chemistry Letters 12 (23), 5639-5643 (2021).