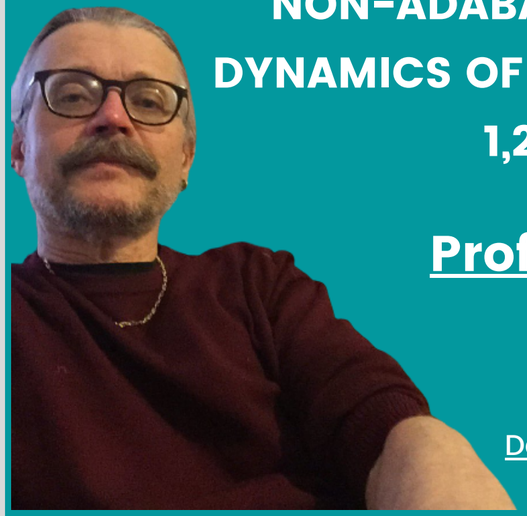
"NON-ADABATIC CHEMILUMINESCENT DYNAMICS OF THE METHYL-SUBSTITUTED 1,2-DIOXETANES"



Prof. Dr. Roland Lindh

The Quantum Chemistry Group

Roland Lindh Group

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Uppsala, Sweden

February 05, 2021 (Friday)

12pm (BRT time) - Google Meet

ORGANIZATION:

Prof. Dr. Antonio Carlos Borin

Instituto de Química, Universidade de São Paulo (USP), SP, Brazil

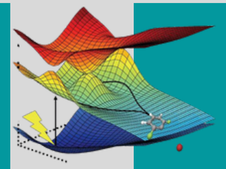
INFORMATION AND REGISTRATION:

ancborin@iq.usp.br

Registration: send a message to ancborin@iq.usp.br

with the words "Roland Lindh – Virtual" on the "subject"

Deadline: February 03, 2021 (Wednesday), 06pm (BRT time)



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ABSTRACT

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That the origin of chemi- and bioluminescence is a non-adiabatic process originating from the breakage of a peroxide bond is well understood. However, some details in the mechanisms of chemi- and bioluminescence are not well understood. In this lecture we will unravel one of these lesser understood experimental observations. That is, the intriguing and dramatic increase - 0.003 to 0.35 - of the quantum yield of the phosphorescence for the series of 1,2-dioxetane molecules substituted going from none up to four methyl groups. This changes of quantum yield, more than two orders of magnitude, is studied in a series of non-adiabatic surface hopping dynamics simulations using multiconfigurational electron structure theory. The dynamics reveal how the seemingly innocent methyl groups retards the dynamic of the fragmentation process - 1,2-dioxetane thermally fragments to two formaldehyde - in a so-called entropic trap, there by enhancing the interstate crossing efficiency. The lecture will initially give a brief background to the field of chemi- and bioluminescence, followed by the details for the problem and simulations listed above.