VISTA Seminar

Seminar 115

October 28, 2026

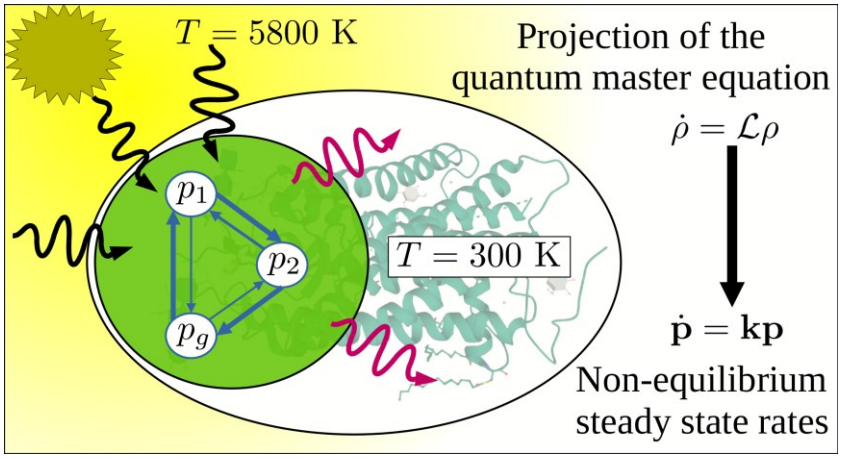
10:00 am – 11:30 am EDT Buffalo / 3:00 – 4:30 pm BST London / 4:00 pm – 5:30 pm CEST Paris / 10 pm – 11:30 pm CST Beijing

TOC:

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Reaction Timescales for Non-Adiabatic Processes in Non-Equilibrium Steady States

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The extraction of characteristic timescales of non-adiabatic processes is essential for understanding complex molecular dynamics. At equilibrium, rate constants can be rigorously related to time-correlation functions through linear-response theory and the fluctuation–dissipation theorem [1]. However, extending this connection to driven open quantum systems evolving toward a non-equilibrium steady state (NESS) remains a largely unresolved challenge.

In this work, we investigate reaction timescales in quantum systems subject to continuous incoherent-light driving and coupled to dissipative environments (see figure below). These systems evolve toward a NESS characterized by a persistent energy flow between distinct reservoirs, leading to dynamical behavior that differs substantially from both equilibrium dynamics and transient dynamics induced by ultrafast excitation [2]. We introduce a projector-based framework [3] that partitions the system Hilbert space into physically relevant configurations, enabling the direct extraction of effective reaction rates under NESS conditions. Applying this framework to a model light-harvesting system, we demonstrate a pronounced dependence of the resulting timescales on the properties of the driving field, highlighting the role of non-equilibrium conditions in shaping quantum reaction dynamics. This approach provides a general framework for characterizing reaction timescales in driven-dissipative quantum systems beyond the equilibrium regime.

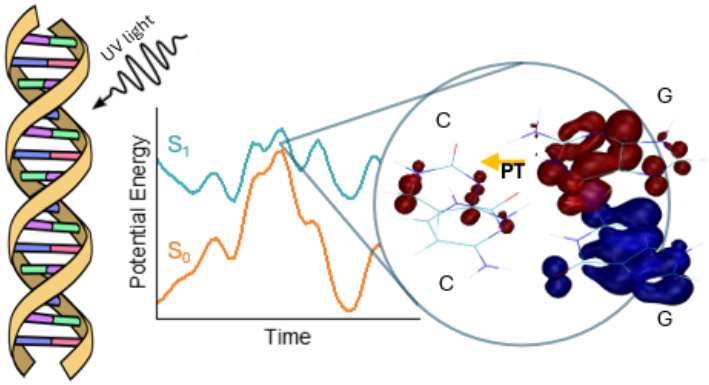
References:

[1] Miller, W. H., Schwartz, S. D. and Tromp, J. W., *J. Chem. Phys.* **1983**, 79, 4889.
[2] Brumer, P. *J. Phys. Chem. Lett.* **2018**, 9, 2946.
[3] Joubert-Doriol, L., Jung, K. A., Izmaylov, A. F., and Brumer, P. *J. Chem. Theory Comput.* **2023**, 19, 1130.

The Hidden Routes of DNA Photostability

Juliana G. de Abrantes,[1]* Josene M. Toldo,[2,3] Mario Barbatti,[3,4] and Marco Sacchi[1]

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DNA's extraordinary resistance to UV-induced damage—essential to the survival of genetic material since prebiotic times—stems from its ability to rapidly and efficiently dissipate energy through damage-free relaxation channels. Multiple decay pathways have been previously identified, but the detailed interplay [1] of these competing mechanisms was not fully understood. In this talk, I will present nonadiabatic excited-state dynamics simulations of alternating and non-alternating stacked cytosine–guanine tetramers. Using fewest-switches surface hopping combined with linear-response TDDFT, we follow the relaxation of initially photoexcited states and analyse the evolving electronic character with various electronic structure descriptors [2].

The simulations reveal an initial population of a G → C charge-transfer state, followed by a diversity of charge redistribution events during the trajectories, culminating with interstrand proton transfer as the dominant relaxation mechanism.

These findings provide a dynamical picture of DNA photostability, in which charge separation, proton motion, and structural fluctuations play a co-dependent role in funneling excitation energy back to the ground state [3].

References:

[1] Martínez-Fernández, L.; Green, J. A.; Esposito, L.; Jouybari, M. Y.; Zhang, Y.; Santoro, F.; Kohler, B.; Improta, R. The photoactivated dynamics of dGpdC and dCpdG sequences in DNA: a comprehensive quantum mechanical study. Chemical Science 2024, 15, 9676−9693.

[2] Plasser, F. and Lischka, H. Analysis of Excitonic and Charge Transfer Interactions from Quantum Chemical Calculations. Journal of Chemical Theory and Computation 2012, 8.8, 2777–2789.

[3] De Abrantes, J. G., Toldo, J. M., Barbatti, M., & Sacchi, M. The Hidden Routes of DNA Photostability: Charge and Proton Transfer in Excited Cytosine–Guanine Tetramers. The Journal of Physical Chemistry Letters 2026, *17*(20), 5709.

How to connect

Alexey Akimov is inviting you to a scheduled Zoom meeting.

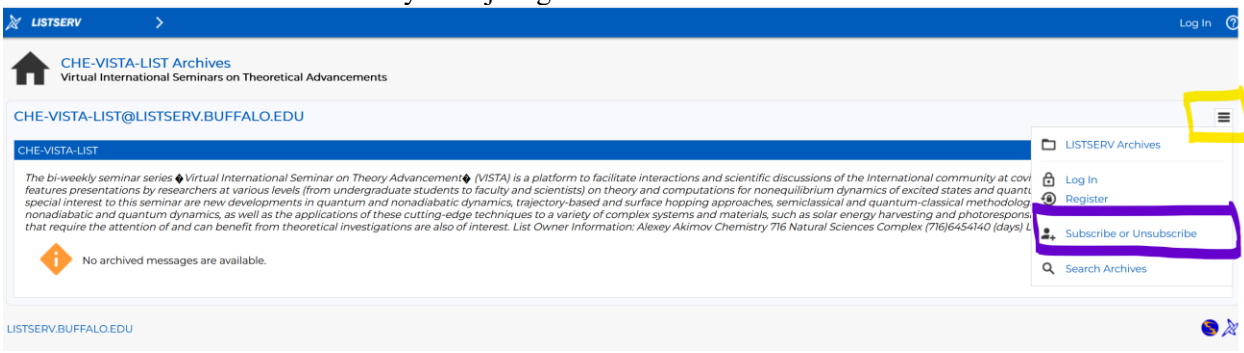
Topic: Seminar #115: Loic Joubert-Doriol and Juliana Abrantes
Time: Oct 28, 2026 10:00 AM Eastern Time (US and Canada)
Join Zoom Meeting
https://buffalo.zoom.us/j/95803595307?pwd=lthL3QrSsEd0wjPijtPKZ9klWdddE5.1

Meeting ID: 958 0359 5307
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2. Click the menu icon in the upper right part of the list (yellow highlight in the picture below)
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2. Quantum Dynamics Hub workspace: https://join.slack.com/t/quantumdynamicshub/shared_invite/zt-mjbhjssx-GGhsbYHxeBMvhmumK_j7LA

C. Gmail calendar:
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