# VISTA Seminar

## Seminar 39

**June 22, 2022**

**10:00 am – 11:30 am EDT / 3:00 – 4:30 BST / 4:00 pm – 5:30 pm Paris**

**TOC:**

1. Presenter 1: Prof. Massimo Olivucci, University of Siena, Italy…..... page 2
2. Presenter 2: Mr. Emanuele Marsili, University of Bristol, UK……..... page 3
3. How to connect……..…. page 4

# On the Origin of the High Quantum Efficiency of Visual Pigments

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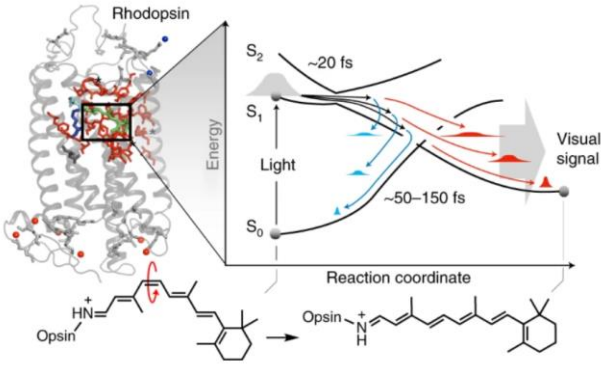


The activation of rhodopsin, the light-sensitive G-protein coupled receptor responsible for dim-light vision in vertebrates, is driven by an ultrafast excited state double-bond isomerization with a quantum efficiency ($\Phi_{cis\text{-}trans}$) of almost 70%. The origin of such a high light sensitivity is not understood. A key unanswered question is whether and how the level of synchronized nuclear (i.e. vibrational) motion controls the $\Phi_{cis\text{-}trans}$ value. Here, we employ hundreds of quantum-classical trajectories to show that, 15 femtoseconds after light absorption, a degeneracy between the reactive excited state and a neighbouring state, causes the splitting of the rhodopsin population into subpopulations propagating with different velocities and leading to distinct contributions to $\Phi_{cis\text{-}trans}$. We also show that such splitting is modulated by the protein electrostatics, thus linking amino acid sequence variations to $\Phi_{cis\text{-}trans}$ modulation.

## References

1. Schnedermann, C.; Yang, X.; Liebel, M.; Spillane, K. M.; Lungtenburg, J.; Fernandez, I.; Valentini, A.; Schapiro, I.; Olivucci, M.; Kukura, P.; Mathies, R. A. Evidence for a vibrational phase-dependent isotope effect on the photochemistry of vision. *Nat. Chem.* 2018, 10, 449-455.

2. Yang, X.; Manathunga, M.; Gozem, S.; Léonard, J.; Andruniów, T.; Olivucci, M. *Nat. Chem.* 2022, DOI: 10.1038/s41557-022-00892-6

# A Theoretical Perspective on the Actinic Photochemistry of 2-hydroperoxypropanal

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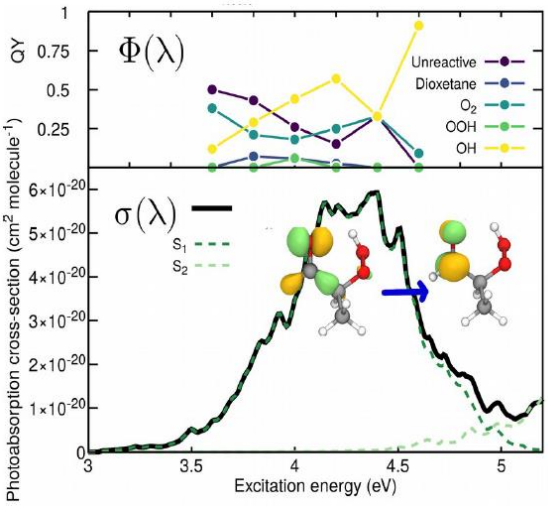



Determining the chemical composition of the Earth's troposphere and its evolution over time is crucial for shaping the political and societal decisions regarding air pollution and global warming. Chemical processes related to volatile organic compounds (VOCs) are of particular relevance in this context. Presently used chemical mechanism models - encompassing experimental and theoretical data for many ground-state reactions of VOCs - allow estimating the outcomes of VOCs oxidation reactions. Interestingly though, the role of light-induced, excited-state processes is still largely unexplored and photochemical reactions of transient VOCs are mostly neglected in predictive atmospheric models.

One family of VOCs formed in isoprene oxidation reactions are α-hydroperoxycarbonyls. Since experimental studies on these transient molecules are hardly feasible, we have employed high-level quantum chemical methods to fully characterize the photochemistry of the 2-hydroperoxypropanal (2-HPP). Using the nuclear ensemble approach we calculated the photo-absorption cross-section (σ(λ))[1, 2] while we resorted to nonadiabatic molecular dynamics to determine the wavelength-dependent photolysis quantum yield (Φ(λ)). These two ingredients, together with the solar actinic flux (F(λ)), allow us to predict the photolysis rate constant J, a crucial piece of information required by predictive chemical mechanism models.

## References

[1] Prlj A., et al., *The Journal of Physical Chemistry Letters*, **11** 5418-5425 (2020).
[2] Prlj A., Marsili E., et al., *ACS Earth and Space Chemistry*, **6** 207-217 (2022).

# How to connect

Alexey Akimov is inviting you to a scheduled Zoom meeting.

Topic: VISTA, Seminar 39
Time: Jun 22, 2022 10:00 AM Eastern Time (US and Canada)

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