DIPARTIMENTO DI CHIMICA E CHIMICA INDUSTRIALE

UNIVERSITÀ DI PISA

POLO S. CATALDO - VIA MORUZZI 13, PISA

Massimo Olivucci

Department of Biotechnology, Chemistry and Pharmacy, University of Siena, Department of Chemistry, Bowling Green State University, OH, USA

On the Origin of the High Quantum Efficiency of Visual Pigments

Lunedì 15 novembre 2021, ore 14.30, aula F/022

Abstract

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 neighboring 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.

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. in press.

Everyone is cordially invited

Lorenzo Di Bari