

# LE DEPARTEMENT DE CHIMIE PHYSIQUE

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## **CONFERENCE**

Intitulée

# ULTRAFAST CHARGE TRANSFER DYNAMICS IN BIOIMAGING DYES, MACROMOLECULAR RECEPTORS, AND DE NOVO PROTEINS

donnée par

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le MARDI 25 NOVEMBRE 2025 à 16h30

SALLE 1S081 Sciences III

30 quai Ernest-Ansermet ou 4 bld d'Yvoy

Responsable : Prof. Ricardo Fernández-Terán

#### Abstract:

Nile Red is a fluorescent dye used extensively in bioimaging due to its strong solvatochromism. The photophysics underpinning Nile Red's fluorescence have been disputed for decades, with some studies claiming that the dye fluoresces from two excited states and/or that the main emissive state is twisted and intramolecular charge-transfer (ICT) in character as opposed to planar ICT (PICT). A combined experimental and theoretical study was used to unravel the mechanism of Nile Red's fluorescence, demonstrating that the molecule is not dual fluorescent, and emission occurs from the Franck-Condon PICT state.<sup>1</sup>

Synthetic carbohydrate-binding proteins (lectins) are used as key tools in medicine to monitor glucose concentrations. Prior studies of a supramolecular synthetic lectin comprised of two cofacial anthracene moieties show that binding glucose increases the lectin's intrinsic fluorescence yield.<sup>2</sup> Our ultrafast measurements reveal that intramolecular charge-transfer within these lectins governs their fluorescence behaviour. Glucose binding to the supramolecular structure alters the associated non-radiative rate and thus underpins the macromolecule's key intrinsic functional emissive properties.

Using ultrafast two-dimensional electronic spectroscopy with sub-8 fs time resolution and >150 nm bandwidth,<sup>3</sup> we probed the photoinduced dynamics of a model *de novo* hemebinding protein, 4D2, inspired by the cytochrome-*bc*<sub>1</sub> complex important in respiring bacteria.<sup>4</sup> Our experiments on the synthetic protein reveal that ultrafast Histidine-Iron bond cleavage is the main non-radiative decay pathway, and that studies of the well-defined artificial protein help to resolve controversy surrounding the non-radiative relaxation in the counterpart natural system.

## References

- <sup>1</sup> C. Gajo, D. Shchepanovska, J.F. Jones, G. Karras, P. Malakar, G.M. Greetham, O.A. Hawkins, C.J.C. Jordan, B.F.E. Curchod, and T.A.A. Oliver, *J. Phys. Chem. B* **128**(47), 11768–11775 (2024).
- <sup>2</sup> C. Ke, H. Destecroix, M.P. Crump, and A.P. Davis, *Nat Chem* **4**(9), 718–723 (2012).
- <sup>3</sup> C. Gajo, C.J.C. Jordan, and T.A.A. Oliver, J. Phys. Chem. A **129**(15), 3537–3551 (2025).
- <sup>4</sup> G.H. Hutchins, C.E.M. Noble, H.A. Bunzel, C. Williams, P. Dubiel, S.K.N. Yadav, P.M. Molinaro, R. Barringer, H. Blackburn, B.J. Hardy, A.E. Parnell, C. Landau, P.R. Race, T.A.A. Oliver, R.L. Koder, M.P. Crump, C. Schaffitzel, A.S.F. Oliveira, A.J. Mulholland, and J.L.R. Anderson, *Proc. Natl. Acad. Sci. USA* **120**(31), e2306046120 (2023).