

Ultrafast Multidimensional Spectroscopy: A Window into Proton-Coupled Electron Transfer and its Control

Ricardo J. Fernández-Terán*

Abstract: This perspective discusses the application of multidimensional spectroscopies in the study of electron transfer, proton transfer, and proton-coupled electron transfer (PCET) processes in the excited state. By addressing vibrational modes intimately tied to the reaction coordinate, these techniques aim to probe, perturb, and ultimately steer photochemical reactions. Simultaneously, multidimensional spectroscopies will provide unparalleled insight into these processes, accessing observables not available to conventional ultrafast spectroscopy. Altogether, this approach allows us to move beyond simple observation towards active manipulation of fundamental chemical reactions in the excited state.

Keywords: · Excited states · Multidimensional spectroscopy · Photochemistry · Proton-coupled electron transfer · Ultrafast spectroscopy



Ricardo J. Fernández-Terán began his chemistry studies at the Simón Bolívar University in Venezuela, moving in 2014 to Uppsala University (Sweden), where he received his BSc (2015), and MSc degrees (2016). He obtained his PhD in chemistry from the University of Zurich (Switzerland) in 2021, under the supervision of Prof. Peter Hamm, specialising in time-resolved IR spectroscopy in one and two dimensions.

He then joined the University of Sheffield (UK) with Prof. Julia A. Weinstein as an SNSF Postdoctoral Fellow. There, he studied the IR control of electron transfer reactions and implemented novel techniques like 2D-IR spectroelectrochemistry to investigate transition metal hydrides. In 2023 he joined the University of Geneva (Switzerland) as a postdoc with Prof. Eric Vauthey. The same year, he was awarded an SNSF Ambizione grant to lead his independent research group in Geneva, focusing on ultrafast multidimensional spectroscopy and IR control of PCET reactions, the design, synthesis and study of novel photoactive complexes, and (photo)catalytic small molecule activation.

1. Introduction

Proton-coupled electron transfer (PCET) is an ubiquitous and fundamental class of chemical reactions, in which the transfer of an electron is coupled to the transfer of a proton. PCET can proceed *via* sequential or fully synchronous pathways and is distinct and often energetically favoured over uncoupled electron or proton transfer (Fig. 1a). PCET is at the heart of many chemical and biological processes, playing a central role in enzymatic catalysis, photosynthesis, and catalytic small-molecule activation.^[1–9]

A comprehensive understanding of PCET in terms of its kinetics, thermodynamics, and underlying quantum mechanical principles is therefore of great importance towards disentangling natural energy transduction systems, and for the rational design of synthetic catalysts for renewable energy applications in artificial

photosynthesis.^[10–12] Ultrafast spectroscopy has emerged, in this context, as an indispensable tool for elucidating the inner workings of light-induced PCET reactions – often taking place on timescales ranging from femtoseconds to nanoseconds, thus placing them directly within the horizon of ultrafast laser techniques.^[13] With the help of ultrafast spectroscopic methods like transient absorption/pump–probe spectroscopy, (Fig. 1b) and multidimensional spectroscopies (*vide infra*), the dynamics of PCET may be resolved, allowing us to distinguish between concerted and sequential mechanisms, potentially identifying short-lived intermediates, and directly measuring key kinetic parameters like rate constants and kinetic isotope effects. This temporal resolution provides a direct window into the reaction coordinate, allowing for the experimental validation of theoretical models and offering unprecedented insight into the fundamental coupling between nuclear and electronic motion that defines PCET. To gain a better understanding of PCET, we can also focus on electron transfer (ET) and proton transfer (PT) – its constituent elementary processes. Indeed, perturbing or controlling these processes can prove fundamental for understanding PCET itself.

2. Controlling the Reaction Outcome with Light

Rather than just passively probing the outcome, light can also be used to modify the outcome of a photochemical reaction. A pioneering approach towards controlling excited-state reactivity, known as ‘*coherent control*’, utilises shaped excitation pulses to create tailored wavepackets.

This method relies on the manipulation of quantum-mechanical pathways in the excited state to steer the system towards a desired outcome.^[14–19]

A more recent and complementary approach involves the incoherent excitation of specific vibrational modes from the initial state. Rather than generating a tailored wavepacket, the excited state is simply populated as usual and perturbed afterwards. In these so-called ‘*IR control*’ experiments (Fig. 2), a UV/Vis pulse first triggers the electron transfer reaction (UV_{pump}), and a

*Correspondence: Dr. R. J. Fernández-Terán, E-mail: Ricardo.FernandezTeran@unige.ch

Department of Physical Chemistry, University of Geneva, 30 Quai Ernest-Ansermet, CH-1205 Geneva, Switzerland.

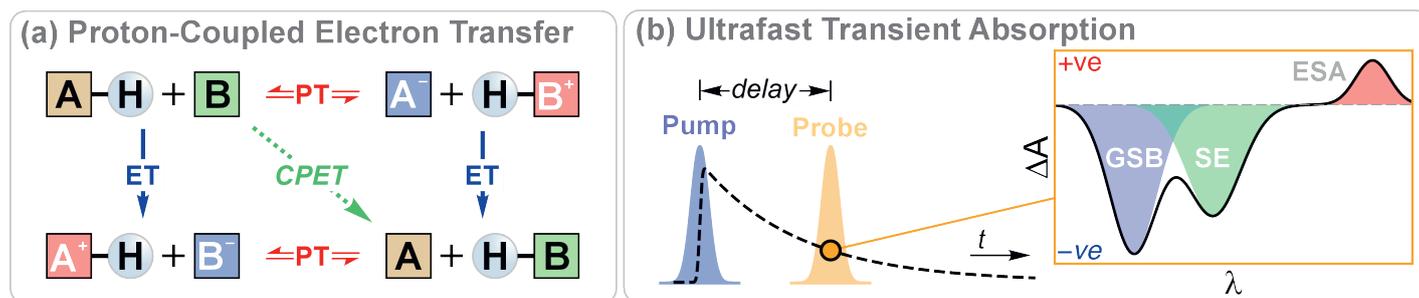


Fig. 1. (a) Schematic representation of proton-coupled electron transfer reactions. ET = electron transfer, PT = proton transfer, CPET = concerted proton–electron tunnelling; (b) Schematic representation of transient absorption spectroscopy: a pump pulse initiates a photochemical reaction, and a probe pulse detects the spectral changes after a controlled delay. Measuring at several delays provides the temporal information. The inset shows a schematic transient absorption spectrum with its potential contributions: GSB = ground-state bleach, SE = stimulated emission, ESA = excited-state absorption.

subsequent, carefully timed narrowband infrared pulse (IR_{pump}) selectively excites specific vibrational modes of the nascent post-charge-transfer state. By depositing energy into specific chemical bonds or a vibrational mode coupled to the reaction pathway, this IR excitation can alter branching ratios with up to 100% efficiency, thereby exerting active control over the final products.^[20–24]

The systems which are intrinsically suitable for IR control typically have a donor–bridge–acceptor (D–B–A) architecture, as the extent of the charge/electron transfer can be monitored independently from the perspective of either moiety by choosing a suitable probing region (in either the UV/Vis or mid-IR ranges), and the bridge can be designed to possess strong, specific and local mid-IR absorption signatures.

Lately, the element-specificity of ultrafast X-ray spectroscopy has also been used to gain deeper insights into photoinduced electron transfer reactions and their control, an active and promising field that we are aiming to explore in the near future.^[13]

Key factors that play a role in determining the success and/or feasibility of IR control include the vibrational lifetime, the extent of (de)localisation of a given vibrational mode, and the directionality of the flow of vibrational excitation in the molecule – often significantly different between the ground and excited states. These and other aspects can be investigated in depth by using multidimensional spectroscopic methods such as two-dimensional infrared spectroscopy (2D-IR) and two-dimensional vibrational–electronic spectroscopy (2D-VE).^[25,26]

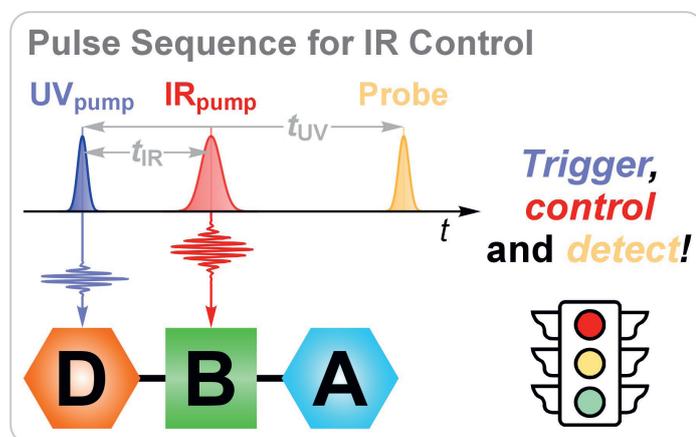


Fig. 2. Pulse sequence for ‘IR control’ experiments: a first UV/Vis pump excites the (electron) donor, followed by a narrowband IR pump which vibrationally excites the bridge. The changes in the spectra are monitored with a broadband UV/Vis or mid-IR probe pulse. The extent of charge/electron transfer is monitored from the viewpoint of the acceptor (A), the donor (D) and/or the bridge (B).

3. Ultrafast Multidimensional Spectroscopy

3.1 Why do we Need a Second Dimension?

Time-resolved spectra are intrinsically ‘two dimensional’ since they constitute an array of spectra sorted by time delays between the pump and probe pulses, however, two-dimensional spectroscopy in this context implies the existence of two complementary frequency axes. Typical transient absorption spectra are often collected with a narrowband pump pulse and a broadband probe. The use of a narrowband pump pulse limits the time resolution (because of the duality between time duration and spectral bandwidth), and it does not exploit the full potential of third order nonlinear spectroscopy.^[25]

One approach to build a 2D spectrum is to vary the excitation wavelength in small steps using a narrowband pump pulse (Fig. 3a). The series of transient spectra obtained in this manner – for a fixed pump–probe delay – can be stacked together (after scaling to account for potentially different pump intensities) to build a 2D map with two frequency (wavelength) axes: the pump frequency (ω_{pump}) and the probe frequency (ω_{probe}). Using this approach, Hamm, Lim and Hochstrasser reported in 1998 the first two-dimensional vibrational spectrum of the amide I mode of a peptide,^[27] a breakthrough representing the birth of two-dimensional spectroscopy in the vibrational (IR) regime.

Whilst 2D-NMR spectra are routinely used nowadays to characterise reaction products, 2D spectroscopy in the optical regimes (UV/Vis/NIR, mid-IR and THz) is significantly more difficult to implement due to the difficulties in controlling the phase and amplitude of optical (light) fields and due to the generation requirements for each region.

Using a broadband pump pulse, the time resolution of a pump–probe experiment can be further increased and pushed to its limit, albeit at the cost of losing the information on ω_{pump} . This limitation can be overcome if the broadband pump pulse is interfered at the sample with a time-delayed copy of itself, and a series of transient absorption spectra are collected for each delay (Fig. 3b). A subsequent Fourier transform along the time delay between the two pump pulses (t_1 or *coherence delay*) allows us to retrieve the pump/excitation frequency axis ($\omega_{\text{pump}} = \omega_1$). The probe axis is typically given by the spectrometer, or by Fourier transform along the signal delay (t_3 or *detection delay*), and hence $\omega_{\text{probe}} = \omega_3$. The delay between the second pump and the probe pulse is known as the *population delay* (t_2).

Recent advances, including the advent of more robust and stable laser sources operating at higher repetition rates, have significantly reduced the acquisition time required for a 2D spectrum, leading to significant developments like the combination of ultrafast multidimensional spectroscopies with microscopy and other techniques.^[28–30]

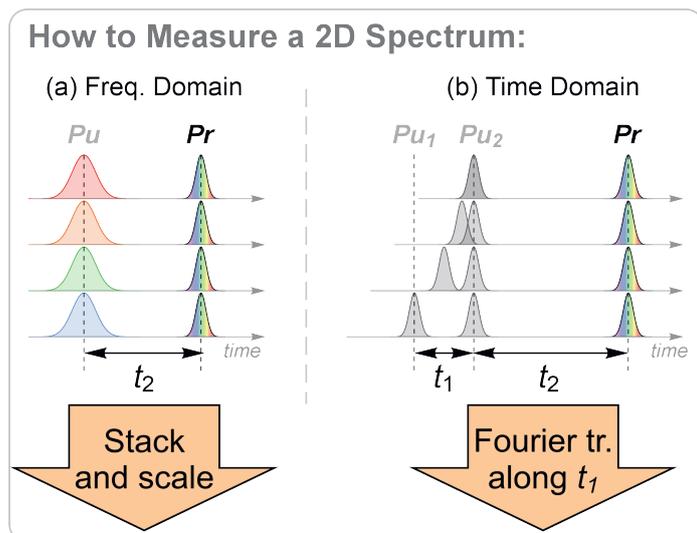


Fig. 3. Pulse sequences required to obtain 2D spectra in the (a) frequency domain, and (b) time domain. In the frequency domain, the central frequency of a narrowband pump pulse is varied, and the corresponding spectra are stacked. In the time domain approach, two broadband pump pulses interfere at the sample with a varying delay (t_1), which after Fourier transform yields the pump spectral axis.

3.2 Information Content of a 2D-IR Spectrum

We shall now focus on the intricacies of 2D-IR spectroscopy, and in particular, on the information content of a 2D-IR spectrum. First, the 2D-IR spectrum of an isolated vibrational band (Fig. 4) contains two contributions of opposite signs: the negative bleach and stimulated emission, observed at $(\omega_{01}, \omega_{01})$; and the positive excited-state absorption, observed at $(\omega_{01}, \omega_{01}-\Delta)$, where Δ is the anharmonicity (*i.e.* the difference between ω_{12} and ω_{01} , see Fig. 4).^[25] The coordinates correspond to $(\omega_{\text{pump}}, \omega_{\text{probe}})$. This double peak feature is absent in typical 2D-NMR spectra, where each resonance shows only the first contribution since the nuclear spin can be considered as a system with infinite anharmonicity.

In close analogy to 2D-NMR spectra, a 2D-IR spectrum may contain cross peaks (each of them however appearing as a positive/negative pair). This in turn allows 2D-IR spectroscopy to distinguish anharmonic vibrational couplings, population transfer and chemical exchange.^[31,32] The 2D line shapes, in particular, reveal unique information which is hidden in the

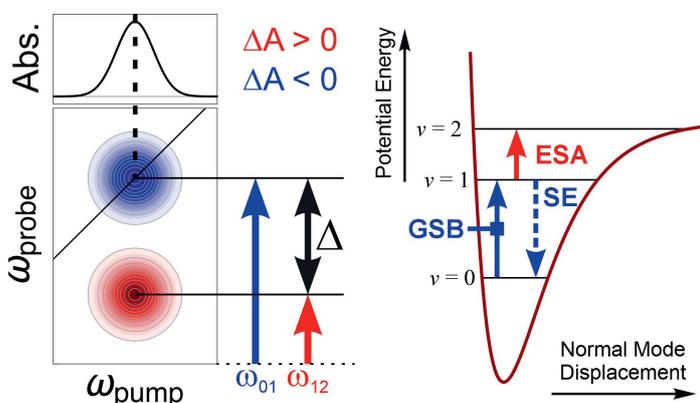


Fig. 4. Basic anatomy of a 2D-IR spectrum (*left*): the fundamental transition is bleached along the diagonal (blue, negative sign), and an anharmonically shifted excited-state absorption (red, positive sign) appears, typically at lower probe frequencies, as expected from a Morse-type potential (*right*). The separation between the two yields the anharmonicity (Δ).

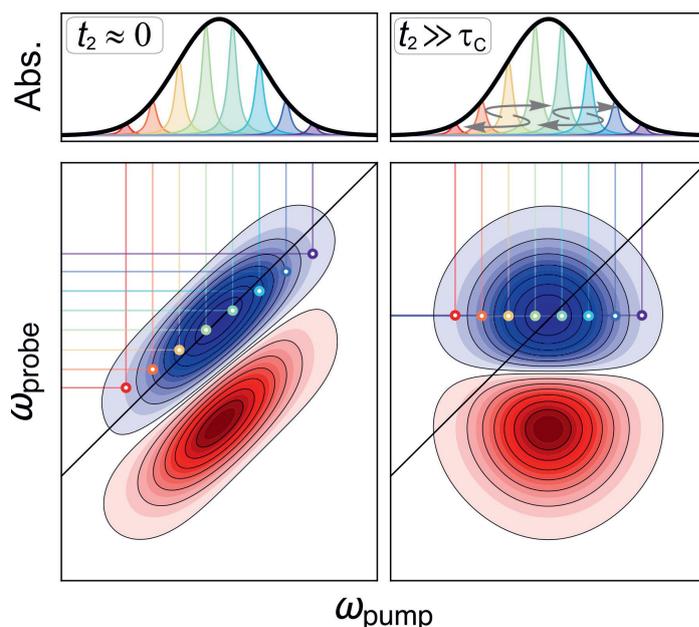


Fig. 5. Spectral diffusion and its impact on the 2D-IR line shapes: For an inhomogeneously broadened system, the decay in the initial correlation (τ_c) leads to an averaging of the probing frequency at long population delays. The lines illustrate schematically the positions of the excited (vert.) and detected (horiz.) sub-populations.

linear (absorption) spectra about the timescale of solvent–solute interactions and fluctuations (Fig. 5).^[25]

4. From IR Control to Multidimensional Spectroscopy: A Window into PCET

Our first step towards expanding the concept of IR control to other excited-state processes began with the examination of systems which undergo symmetry breaking in the excited state.^[33–36] Excited-state symmetry breaking (ES-SB) involves the localisation of charge in an otherwise symmetric molecule (in our case, a D–A–D system), as a consequence of solute–solvent and other interactions.

We employed *transient* 2D-IR spectroscopy to obtain a 2D-IR spectrum of the excited-state species as a function of solvent polarity. The pulse sequence for time-domain transient 2D-IR (t2D-IR) largely resembles that of the IR control experiment (Fig. 2), except that the narrowband IR pump pulse is replaced by a broadband pulse pair as in Fig. 3b. The UV/Vis pulse is thus used to generate the excited state species of interest, followed by a conventional 2D-IR pulse sequence.^[37–39]

We obtained precious information on the aspects discussed in section 3.2, and were able to fully characterise the excited state vibrational landscape of the bridge modes in a molecule undergoing ES-SB. A manuscript reporting on the findings of this investigation is currently under preparation.

In the same context, it is worth noting our previous work on donor–bridge–acceptor systems based on Pt(II) *trans*-bisacetylides.^[40] Isotopic (^{13}C) labelling of both acetylene carbon atoms on either the donor, the acceptor, or both sides of the molecule, allowed us to elucidate the changes in vibrational couplings and the flow of energy transfer in the molecule, using the ground-state 2D-IR spectra as a framework to understand the excited-state vibrational landscape. It was in these systems where the original IR control effect was reported.^[21] The complexes which were ^{13}C -labelled only on one side of the molecule showed close to complete mode localisation, and negligible vibrational energy transfer between the donor/acceptor acetylide moieties, offering a valuable molecular design criterion to retain the

bond specificity of vibrational modes in a large molecule. With the help of t2D-IR spectroscopy, we will determine whether IR control of excited-state symmetry breaking is feasible, and on the implications of mode localisation to this end.

Our current efforts in this direction involve the synthesis and study of ¹³C-labelled molecules which undergo ES-SB, the study of symmetric Pt(II) *trans*-bisacetylides and Au(I) acetylides with substituents of different donor strengths and conjugation lengths,^[41] and the study of the effect of remote substitution in steering the character of the excited state of a metal complex.^[42–44] We are also examining other D–B–A architectures with t2D-IR spectroscopy, with a particular focus on the role of Fermi resonances on the potential for IR control of electron transfer processes. Finally, as we have recently shown,^[31] transition metal hydridocarbonyls are an ideal playground to explore these and other ideas, which are the current and upcoming focus of our research. In the future, we hope to combine complementary probing ranges (from the THz and the mid-IR to X-rays) with multidimensional techniques to fully characterise the excited state dynamics of the systems of interest.

5. Conclusions and Outlook

In this perspective, we have discussed multidimensional spectroscopies (with a particular focus on 2D-IR spectroscopy) and their application towards the study of electron transfer, proton transfer and PCET reactions. By directly addressing vibrational modes which are intimately related to the reaction coordinate, we aim to probe, perturb, and ideally steer the outcome of electron transfer, proton transfer and PCET reactions in a vast array of systems, ranging from organic to organometallic and supramolecular D–B–A architectures. By combining the concepts of IR control and multidimensional spectroscopies, we aim to gain the utmost insight on these processes, leading to an in-depth understanding of the inner workings of said phenomena, bringing us closer to the dream of controllable light-induced reactivity.

Acknowledgements

I thank my PhD student, Joseph Kölbel, for his hard work and enthusiasm. I also acknowledge my mentors, Prof. Julia A. Weinstein, Prof. Peter Hamm, and the previous and current contributors to the work discussed herein, amongst them, Dr. Jan Helbing, Dr. Laurent Sévery, Dr. Jeannette Ruf, Aleksandra Dimitrieva, William Stewart, Dr. Iona Ivalo, Dr. James Shipp, Dr. Martin Appleby, Estefanía Sucre-Rosales, and Alena Chernikova. Our collaborators and partners including Prof. Thomas Teets, Prof. Claude Piguet, Prof. Steven P. Nolan, and Dr. Maxime Poncet are also acknowledged. The invaluable support and mentorship of Prof. Eric Vauthey who kindly hosts our research group at the University of Geneva, is gratefully acknowledged. Financial support from the University of Geneva, from Johnson Matthey plc. (PGM Award Scheme), and from the Swiss National Science Foundation (Early Postdoc.Mobility grant P2ZHP2–199422; Ambizione grant PZ00P2–216249) are gratefully acknowledged.

Received: September 15, 2025

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