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<tr>
<td>Title</td>
<td>Instrumentation and science from the final years of Ahmed Zewail’s second generation ultrafast electron microscopy lab</td>
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Abstract:

In the effort initiated by Ahmed Zewail to develop ultrafast electron microscopy into a powerful tool for directly observing the dynamics of matter with unprecedented resolutions in space and time, the Zewail labs at Caltech were tasked with creating the requisite instrumentation and using it to investigate as broad a range of applications as possible. In this talk, I will give some examples of both of these aspects of the work carried out in the second generation ultrafast microscopy laboratory (UEM-2) in the final years of the Zewail group.
Abstract:

This talk will review the development of ultrafast gas-phase electron diffraction (UGED) in Dr. Zewail’s group at Caltech and how we overcame several major challenges to realize the first picosecond (ps) UGED, including the determination of time zero point and the extraction of transient molecular structures in photo-induced chemical reactions. Using UGED, the structure of CF2 generated in the photodissociation of CF2I2 molecule has been determined with high accuracy in the ps time resolution. For C2F4I2 molecule, the time evolution of shirt-lived intermediate in the course of a chemical reaction has been monitored directly with UGED. The elimination of two iodine atoms was shown to be stepwise with the second iodine dissociation time of 17 ± 2 ps.

References

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Title : 4D Electron Microscopy: Applications in Materials Science

Abstract:

Over the last decade, 4D electron microscopy that is capable of imaging ultrafast dynamics in both space and time, has made enormous progress, opening a large variety of applications in chemistry, physics, materials science and biology. In this conference, I will present our recent results, focusing on the irreversible dynamics from a single nanoscale object in the field of materials science. Examples for applications are given, including studies of the phase reaction and motion dynamics of nanostructures. The involved processes were initiated with a laser excitation pulse while a single electron pulse was used to image the transient features by using single-pulse mode of 4D electron microscopy. The mechanisms that account for the observed phenomena will be discussed.
In this talk we will discuss the applications of femtosecond time-resolved photofragmentation spectroscopy to ultrafast photoionization-induced molecular ion chemistry. In this method, a femtosecond pump pulse first produces an ensemble of positive ions via photoionization of the neutrals. Owing to the fact that the molecular nuclear and electronic structures often exhibit significant changes upon removal of an electron, vertical femtosecond photoionization can prepare ionic states far away from the global equilibrium configuration of the system. The initially prepared ionic states then evolve according to the nature of the ionic system, and a delayed probe pulse then brings the evolving ionic system to higher excited states that ultimately lead to fragmentation. The ionic dynamics can be detected by monitoring either the parent-ion depletion or fragment-ion formation as a function of the pump-probe delay time, provided that the probing transition varies along the reaction coordinate. This fs-pump-probe photoionization-photofragmentation (PI-PF) scheme is simply the time-domain version of ion photofragmentation spectroscopy and is most suitable for studying photoionization induced ion chemistry in ultrafast time scales. In some specific molecular systems, photoionization-induced reactions correspond to important elementary steps in chemistry. In this talk we will try to discuss applications of this technique to photoionization-induced twisting isomerization in azobenzene cation [1], intermolecular proton transfer in phenol-ammonia complex cation [2,3], and charge transfer in bi-functional molecular cations.

References
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<td>Title</td>
<td>Ultrafast X-ray and optical studies of materials and molecular systems</td>
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Abstract:

We will review recent work on the ultrafast dynamics of molecular and materials systems using various tools developed by our group: 1- and 2-dimensional deep-UV spectroscopy, Vacuum ultraviolet Photoelectron spectroscopy and hard X-ray spectroscopy. We will discuss the connections between these various observables and how they allow a full picture of the on-going dynamics.
Molecules under laser excitation exhibit extreme behavior. Two examples of such behavior will be presented. Recent work from our group led to the discovery that the formation of H$_3^+$ following strong-field photodissociation of methanol is preceded by the formation of neutral H$_2$ molecules that roam the parent ion and extract a proton [Ekanayake, N. et al. Sci. Rep. 7, 4703 (2017)]. In that study, two reaction pathways for the formation of H$_3^+$ under strong-field ionization starting from a doubly-charged methanol precursor were elucidated experimentally and theoretically [Figure 1]. More recently, site-specific details and femtosecond time-resolved dynamics of H$_3^+$ formation have been obtained through a combination of time-resolved mass spectrometry, photoion-photoion coincidence measurements, and ab initio calculations for a series of alcohols. Our findings confirm the mechanisms of this intriguing chemical process involving ultrafast double ionization of the parent molecule leading to the cleavage and formation of three chemical bonds. In condensed phase molecular reactivity can change dramatically with the absorption of a photon because the excited state electronic configuration is different from that of the ground state. The ultrafast dynamics of excited state intermolecular proton transfer from organic protic solvents to a conjugated Schiff base molecule acting as a photobase will be presented. Upon excitation, the Schiff base undergoes a 14-unit increase in pK$_a$, making the excited state pK$_a^* \sim 28$, hence its designation as a “super” photobase. We observe that the proton transfer process is initiated within the timescale of solvent dielectric relaxation, a step coupled with the formation of a partially-transferred proton complex between the base and the solvent prior to the complete proton transfer event.

![Figure 1. The strong-field triggered fragmentation of methanol includes a chemical reaction producing H$_3^+$ and CHO$^+$.](image-url)
Abstract:

In this presentation, I will focus on the functionalization of graphite and graphene using two approaches. A first approach is based on molecular self-assembly at the interface between a liquid or air, and graphite or graphene. I will discuss concepts of nanostructuring emphasizing the effect of solvent, solute concentration and temperature, stimulus-driven self-assembly and self-assembly under nanoconfinement conditions. A second approach is based on grafting molecules on graphite or graphene via covalent chemistry. In addition to a discussion on the functionalization principles, it will be demonstrated how also nanolithography can be used to nanostructure such covalently modified surfaces.

Advanced interface specific methods such as scanning tunnelling microscopy (STM) and atomic force microscopy (AFM) provide structural and other types of information at the nanoscopic level.

Various applications will be presented, including molecule modified graphene field effect transistors.

Combined nanolithographic, covalent and non-covalent functionalization.
Abstract:

Proton transfer is one of the most fundamental processes involved in chemical and biochemical reactions. Great knowledge has been achieved thanks to ultrafast spectroscopy. The excited-state intramolecular proton transfer (ESIPT) reaction generally takes place in the femtoseconds (fs) time scale. During the last three decades, excited-state proton transfer dyes have been much studied, leading to different applications as laser dyes, UV photostabilizers, photoswitches, chemosensors and optoelectronic materials.

In this talk, we show and discuss results of fs time-resolved studies of two 2-(2'-hydroxyphenyl)benzoxazole (HBO) amino derivatives in different media. In these systems, an intramolecular charge-transfer (ICT) process takes place before the ESIPT reaction, affecting the mechanism of this latter reaction. The nature and position of the substituent in the molecular HBO frame modulate the forward/backward ESIPT rate ratio. For instance, when the amino (-NH$_2$) group is in the 6-position of benzoxazole part, the ESIPT process in non-polar solvents is irreversible and relatively slow (1-14 ps), but in polar solvents it becomes reversible and slower (130-170 ps). When the amino group is in the 5-position, the ESIPT reaction times are even slower (~ 1 ns), and follows a reversible mechanism in non-polar solvents. The photobehavior of these dyes and related PT mechanism remarkably change with the solvent nature and position of the amino group in the benzoxazole framework, opening the window for further research and possible applications in other field not yet explored.

Acknowledgements: This work was supported by the MINECO (MAT2014-57646-P, MAT2017-86532-R) and CEI CYTEMA (CEI15-08-5).

* Dedicated to the memory of Prof. Ahmed H. Zewail.

References:
Phys. 2015, 17, 16257-16269.
Abstract:

Despite extensive efforts, the question of how proteins fold still remains unanswered. One practical challenge for experimental characterization of protein folding dynamics and mechanism is that none of the existing techniques is able to capture conformational snapshots of the protein system in question along its folding pathway(s) with the required structural-temporal resolution. In this talk, we will present several newly developed methods that offer the potential to improve our ability to assess various mechanistic details of the folding process of interest and, in some cases, to reveal features of the underlying folding free energy landscape.
The large amplitude and sudden jump dynamics of a hydrogen (H)-bond’s initial rupture and its subsequent formation of an H-bond with a different partner has been argued to well describe the reorientation dynamics in pure water and in aqueous solutions of a wide variety of solutes ranging from simple ions to complex biomolecules. This description is however a classical one for the nuclear motion, and a concern is the possible effect of the quantum character of the light hydrogens’ motions. Here we will recount the main results of our recent efforts to quantify and understand the impact of such nuclear quantum effects on this issue. To this end, we have employed a ring polymer molecular dynamics (RPMD) description for both H₂O and D₂O liquids, with particular emphasis on the chemical reaction perspective for the reorientation process. If time permits, we will also describe our initial efforts to combine RPMD and Grote-Hynes theory for reaction rate constants. This research is a collaboration with Damien Laage (ENS), David Manolopoulos (Oxford), and several of their students, as to be detailed in the presentation.
Abstract:

A grand challenge for quantum physics in the 21st century is a deeper understanding of the complex correlations that arise among many strongly interacting quantum objects, be they electrons, atoms, or photons. Inspired by Professor Ahmed Zewail, I will present an overview of some startling advances in quantum physics over the past three decades. I will draw extensively from examples in which single atoms and photons serve as Quantum Lego Blocks to build larger quantum systems with new functionalities, including an eventual Quantum Internet.
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Title : Direct Visualization of Plasmonic Acoustic Vibration of Single Nanorods in Real Space and Time

Abstract:
With advances in spatial resolution reaching the atomic scale, 2 and 3 dimensional (D) imaging in transmission electron microscopy (TEM) has become an essential methodology in various fields of research providing static structural information. Now it has become possible to integrate the ultrahigh temporal resolution (fourth dimension) to the 3D spatial resolution of TEM. Here, presented is the concept and recent application of time-resolved imaging in ultrafast electron microscopy (UEM), which made it possible to directly visualize a single gold nanorod (Au NR) undergoing plasmonic-acoustic vibration of sub-nanometer amplitude and picosecond period, upon femtosecond-pulsed light excitation for the first time. The unique integration of a direct electron detection camera to ultrafast electron microscopy in combination of achieving control over the quality of pulsed electron beam enabled the unprecedented spatiotemporal resolutions with selective and characteristic vibrations of a single Au NR being unveiled in contrast to conventional optical spectroscopic measurements on ensembles.

References
Abstract:
Most systems in nature---including living organisms---are not at equilibrium. Here, I show that the equilibrium Boltzmann distribution is a special case of a general distribution that governs stochastic systems, even those that are driven far from equilibrium. The general distribution is shown to be a voltage equation in which the constituent parts can be seen as resistors, batteries, node voltages and path currents, which can be directly mapped to equilibrium rate constants, driven rate constants, probabilities and probability flows, respectively. By analyzing nonequilibrium systems as circuits, the theory provides a unified framework to simplify/modularize complex systems into essential collective variables. Applying the theory to a set of common biochemical systems, simple performance limits are derived, and experimental data is used to show that living systems operate near those limits. The generalized Boltzmann distribution is also used to derive two universal relations: (1) the maximum efficiency of molecular engines and (2) the reciprocal relation between driving one part of a system and the response (gain) in another.
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<th>Zhi Heng Loh (presented by Zhengrong Wei)</th>
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<td>Title</td>
<td>Femtochemistry induced by intense laser fields</td>
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**Abstract:**

Strong-field laser-molecule interaction forms much of the basis for initiating and probing quantum dynamics on ultrashort timescales. While recent efforts have primarily focused on elucidating electron dynamics, intense laser fields also invariably trigger coherent vibrational motion and bond dissociation in molecules. In this talk, I will provide selected examples from our recent studies of ultrafast molecular dynamics of strong-field-ionized iodoalkanes probed by differential soft X-ray absorption spectroscopy. Monitoring the iodine 4d core-level absorption at ~50 eV allows the freeze-frame capture of C–I bond dissociation as a function of time and reveals the formation of various dissociative ionization products. Analysis of the vibrational wave packet dynamics disentangles the relative contributions from R-selective depletion and bond softening to the generation of vibrational coherences in the neutral species, reveals multimode vibrational wave packet motion in the parent ions, and directly furnishes vibronic coupling strengths involving core-level transitions. Our results shed light on the elementary ultrafast dynamics that accompany the interaction of intense laser fields with polyatomic molecules.
Abstract:

Singlet fission plays a prominent role in raising the quantum efficiency of organic solar cells. In this overall spin-conserved process two molecules in the triplet state \( T_1 \) are formed by investing just one photon. Acenes with four or more benzene-rings are known to undergo singlet fission and are attractive compounds to develop new chromophores with promising photo-physical-chemical qualities. TIPS-pentacene, as a soluble derivate of pentacene, serves here as starting point and has been studied by means of ultrafast transient absorption measurements and more complex pump-depletion-probe arrangements with high time resolution.[1,2] The obtained detailed picture of the excited state dynamics of TIPS-pentacene presents an excellent reference for studying structure-function relationships of acene derivatives. For example, by systematically modifying the structure by nitrogen to carbon substitution or halogen to hydrogen substitution the influence on the triplet formation can be analyzed. The chemical modification can accelerate singlet fission in the aza-derivative by almost a factor of two. A faster relaxation from the singlet to triplet manifold implies a higher efficiency, because other relaxation channels are avoided.[3]

Figure 1: a) Structure of N-substituted Acenes studied: phenazinothiadiazoles molecules (TDT, TDCl4, TDF4); b) Thin film absorption spectra show a 160 nm shift of phenazinothiadiazoles molecules with regard to TIPS-Tr and overlap absorption of TIPS-Pn nicely; c) fs dynamics of TDCL4 shows sub-picosecond evolution indicating SF.

References
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<th>Author(s)</th>
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<td>Title</td>
<td>Time-Resolved Frequency-Comb Spectroscopy of Gas Phase Free Radical Reactions</td>
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Abstract:

Professor Zewail's vision of femtochemistry was to use ultra-fast lasers to study the reactions of reactive intermediates in the time domain. Now the advent of optical frequency comb lasers allows one to use ultra-fast lasers for real-time frequency-domain spectroscopy, taking advantage of the phase coherence of stabilized ultra-fast lasers to provide broad spectral coverage, enhanced sensitivity and high spectral resolution in the frequency domain. Frequency combs overcome the limitations of conventional spectral multiplexing techniques such as broad-band cavity enhanced absorption spectroscopy and step-scan FTIR, which allow one to observe the time-resolved transient absorption spectra of reactants, intermediates and products over a wide spectral band, but with limited spectral and time resolution, and low sensitivity. In a collaboration with the Jun Ye group at Boulder, we have demonstrated the application of frequency comb spectroscopy to the high sensitivity, time-resolved detection of reactive intermediates in gas phase free radical reactions. We employed the JILA Mid-Infra-Red Time-Resolved Frequency Comb Laser Spectrometer, which couples frequency comb output to an external cavity for cavity enhanced absorption of transient species. I will describe frequency comb spectroscopy experiments using this instrument to detect DOCO and other intermediates in the deuterated analog of the reaction OH + CO. This reaction plays a central role in the chemistry of the atmosphere as well as in combustion and has been a benchmark for studies of reaction dynamics. The sensitivity and bandwidth allow us to observe both trans- and cis-DOCO intermediates and to quantify elementary reaction rates.
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<td>Title</td>
<td>Key Electronic Spectroscopy for Understanding Molecular Recognition and Development of Theranostic Strategies</td>
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Abstract:

The role of optical spectroscopy in the molecular understanding of biomolecular recognition is well-known. The scientific knowledge has immense importance in the plant kingdom (photosynthesis) as well as animal kingdom (diagnosis and therapy of various diseases, called theranostic in short). In the proposed talk, I would discuss the impact of key dynamical events in biological macromolecules duly explored using optical spectroscopy in their function of molecular recognition. The knowledge of the spectroscopy in the development of various nanomaterials for biomedical applications (nanomedicines) would also be highlighted. Finally, our continuous efforts in the development of various spectroscopy-based instruments for the immediate use in various hospitals for the diagnosis of human diseases would be briefed.
Abstract:

If G-quadruplexes form so readily in vitro, Nature will have found a way of using them in vivo' (statement by Aaron Klug over 30 years ago).

During the last decade, four-stranded helical structures called G-quadruplex (or G4) have emerged from being a structural curiosity observed in vitro decades ago, to being recognized as a possible nucleic acid based mechanism for regulating multiple biological processes in vivo. The sequencing of many genomes has revealed that they are rich in sequence motifs that have the potential to form G-quadruplexes and that their location is non-random, correlating with functionally important genomic regions. In will summarize recent evidence for the in vivo presence and function of DNA and RNA G-quadruplexes in various cellular pathways including DNA replication, gene expression and telomere maintenance.
Abstract:

In so elegantly demonstrated 4D electron microscopy, the optimal experimental conditions may be achieved by using a low electron dose per pulse and a high repetition rate to preserve the beam quality while achieving high spatial and temporal resolutions. Meanwhile, for researching complex reactions and macroscopic material transformations, one often faces the strong space-charge limitation to provide adequate electron dose while maintaining the resolutions, provided that the processes in their full expression are less likely reversible. To bring forth the ideas originated from Femtoland to different operating regimes, we adopt a complementary adaptive optics and high-brightness beam ideas to optimize the performance of ultrafast electron microscope. We show that with femtosecond coherent electron pulses thus generated, we can image the macroscopic thermal and interaction-driven phase transitions of correlated electron phases where the dynamical scale-invariant behavior signifies the presence of nonthermal critical points on the excited energy landscape. Such new light-induced critical phenomena could be directly responsible for the creation of hidden phases discovered recently in several quantum materials with technological implications. The combined spatial and temporal resolutions at relatively high electron doses necessary to address this complex phenomenon provides us some confidence about further implementing ultrafast spectroscopy and imaging using different adaptive optical manipulation of high-intensity beams. With that in mind, we will suggest how some of Zewail’s grand vision of making molecular movie in complex systems may be alternatively realized.
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| Title                  | Femtoseconds matter even in non-electron transfer reactions:  
Promoting vibrations and enzyme catalysis |

Abstract:

The mechanisms of enzymes have been studied for many decades, but there remains basic disagreement as to how they achieve such extraordinary rate enhancements. This talk will focus on recent advances in our group aimed at answering just this question. In particular, we have shown over the past decade that rapid, sub picosecond protein motions, built into the protein matrix via evolution are central to the catalytic effect. We have applied these ideas to the concept of enzyme design and with our experimental collaborators have verified this new view of enzymatic action. Recently we have shown that in some cases, these motions modulate electrostatic fields at the active site, and this view harmonizes two divergent schools of thought on enzyme proficiency. The work described involved the development and application of new theoretical methods for the study of chemistry in such complex systems, and this talk will focus on the methods, applications, and experimental verification of the results.
Author(s) : Theis I. Sølling
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Title : Driven dynamics: non-statistical processes on the femtosecond timescale in simple organic molecules

Abstract:

The processes that drive photophysical and photochemical transformations are essentially determined by the shape of the potential energy surfaces in play. If a transition is to be ultrafast the initially activated degrees of freedom have to drive the molecule towards a region of the potential energy surface with a high transition propensity from one electronic state to another. If the coupling between the electronic states involves a reactive degree of freedom it will lead to ultrafast bond breakage (or bond formation). Such driven processes are non-statistical in nature in the sense that not all molecular degrees of freedom have been activated prior to the transition (or reaction) under study. Such an approach to molecular reactivity has its root in the Zewail group and has since been expanded. This presentation will provide examples of molecules where the initial photoactivation leads to highly non-statistical photophysical and photochemical processes. Our work has even revealed examples of complex systems where the initially localized vibration is the only one that remains active on the receiver state and cases where the localization of the excitation energy prevents an otherwise labile bond from breaking.
### Title

Ultrafast Charge Transfer in 2D Semiconductors and Heterostructures

### Abstract:

2D semiconductors, such as transitional metal chalcogenides and black phosphorus, have attracted considerable attention due to fascinating physical properties a wide range of applications in valleytronics, optoelectronics and superconductivity. The interlayer interaction is particularly important in both homogenous few-layer systems and heterogeneous structures formed by “lego” fashion, which underpins the foundation for rational engineering towards unprecedented functionality. In this talk, I will introduce our work on unique interlayer charge transfer mechanism in 2D semiconductor monolayer heterostructures leads to an interesting blinking phenomenon, whereby a bright state emission occurs in one monolayer while a dark state emission occurs in the other, and vice versa. Such correlated blinking can be probed in detail by steady-state and transient spectroscopy measurements, which uncovered an ultrafast charge transfer process ~ 120 fs, providing new platform to study the long-standing puzzling blinking phenomenon in nanomaterials. Secondly, I will present how the charge transfer by a gate modulation breaks the symmetry in a bilayer sample such that a charge-induced second harmonic generation is produced, due to a confined charging in W-atomic plane and a screening effect. This bilayer system can be further modulated by introducing plasmonic structures, from which an ultrafast plasmonic hot carrier injection (~ ps) can lead to symmetry breaking, as such a second harmonic generation is produced. Our study creates opportunity for the ultrafast all-optical control of SHG in an all-optical manner that may enable a variety of applications.

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<td><strong>Title</strong></td>
<td>Dynamics and mechanism of UV-B perception of photoreceptor UVR8</td>
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**Abstract:**

UVR8 (UV RESISTANCE LOCUS 8) proteins are a class of UV-B photoreceptors in high plants. UVR8 is a homodimer that dissociates into monomers upon UV-B irradiation (280 to 315 nm), which triggers various protective mechanisms against UV damages. Uniquely, UVR8 does not contain any external chromophores and utilizes the natural amino acid tryptophan (Trp) to perceive UV-B light. Each UVR8 monomer has 14 tryptophan residues. However, only the epicenter two Trp (W285 W233) residues are critical to the light-induced dimer-to-monomer transformation. Here, combining time-resolved spectroscopy and extensive site-directed mutations, we have revealed the entire dynamics of UV perception to lead to monomerization, including a series of critical dynamical processes of a striking energy-flow network, exciton charge separation and recombination, charge neutralization, salt-bridge zipping and protein solvation, providing a complete molecular picture of the initial biological function.