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# Complex Interactions of Light and Biological Matter: Experiments meet Theory

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# List of Poster Presentations

# Titles with Abstracts

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## Abstract:

# Optically Active Nucleobase Supramolecular Architectures

**Ruth Aizen, Ehud Gazit**

The self-assembly of small organic molecules interacting via non-covalent forces is an important approach towards the construction of highly ordered nanostructured materials. Among various molecular building-blocks, canonical and unnatural nucleobases can undergo non-covalent self-association to form supramolecular architectures. Non-covalent interactions including hydrogen bonding offers great control over the process of molecular organization since it combines selectivity, directionality, reversibility, and cooperativity. Such a unique character is the basis of complex systems found in the biological world. These systems do not only include physiological DNA as the genetic material but also pathological amyloidal aggregates formed by nucleobases in metabolic disorders[1], photonic crystals and more. Therefore, the ability to understand and predict how nucleobases interact among themselves to produce functional assemblies is extremely important.

In the current study we wish to present a library of nucleobases and investigate their intrinsic physio-chemical properties. Specifically, we are interested in screening the optical properties of the nucleobase-related assemblies. This interest is supported by previously reported findings from our group and others that demonstrated intrinsic fluorescence properties of self –assembling Peptide nucleic acids (PNAs) and amyloidal peptides and proteins.[2, 3]

Our preliminary results indicate that nucleobase crystals inherently include unique intrinsic optical properties with some nucleobases demonstrating excitation-dependent emission. Intrinsic fluorescence is supported by fluorescence life-time measurements. This behavior is uncommon in the field of organic supramolecular materials and could have implications in fields such as therapeutics of metabolic disorders and material science.

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# Structuraction in water of fluorene derivatives by mean of colloidal nano-object

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## Abstract

Small organic fluorescent dyes present relevant drawbacks for in vivo applications, as low solubility in aqueous media. Nanotechnologies can provide feasible strategies to disperse in water lipophilic probes . Among these types of nanocarriers, one of the most promising is certainly Quatsomes (QSs), a new class of Small Unilamellar Vesicles (SUVs) formed by the self-assembly in water of a quaternary ammonium surfactant (CTAB) and cholesterol. The main aim of the thesis work was the study of the interaction between QSs and properly engineered dyes, DiC18 and MC18, fluorene derivatives. The use of such dyes is limited by their insolubility in water. Therefore different strategies have been explored to stably disperse DiC18 in water: i) incorporation in QSs membrane (QS-DiC18); ii) dispersion by using CTAB in a concentration above its critical micellar concentration (CTAB-DiC18), iii) formation of dye nanoparticles by reprecipitation (DiC18 NPs). The incorporation in QSs and the dispersion by CTAB lead to the formation of different stable nano-objects, with promising optical properties. In the case of QS-DiC18, the dye forms patches over the membrane of the Quatsomes (Patchy QSs). The high fluorescence quantum yield of QS-DiC18 (which decreases at higher loadings), along with the high colloidal stability, makes these objects good candidates for application in microscopy.

# Intermolecular Energy Transfer In Real Time

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Essential state models (ESM) have been successfully used to describe low-energy optical properties [1, 2, 3] of different classes of charge-transfer (CT) chromophores, namely dipolar (D-A, where D=donor and A=acceptor of electrons), quadrupolar (D-A-D or A-D-A) and octupolar ($A(-D)_3$ or $D(-A)_3$) chromophores. Here we introduce a truly dynamical and non-adiabatic model for resonance energy transfer (RET). More precisely, we consider two different dipolar chromophores, an energy donor ($\mathcal{D}$) and an energy acceptor ($\mathcal{A}$), their main resonating structures being used as electronic basis states and introducing the coupling to one effective molecular vibration per chromophore.

By means of a non-adiabatic dynamical calculation also accounting for energy dissipation, we follow in real time the complete $\mathcal{D}$-to-$\mathcal{A}$ energy transfer process (Fig.1, panel a). Coherent oscillations of $\mathcal{D}^*$ as induced by an ultrafast light pulse are washed-out in a few hundred femtoseconds by fast intramolecular energy dissipation, while the $\mathcal{D}^*$-to-$\mathcal{A}$ energy transfer process takes place in the following few picoseconds (Fig.1, panel b). The whole process is followed through time-dependent fluorescence spectra (Fig.1, panel c).

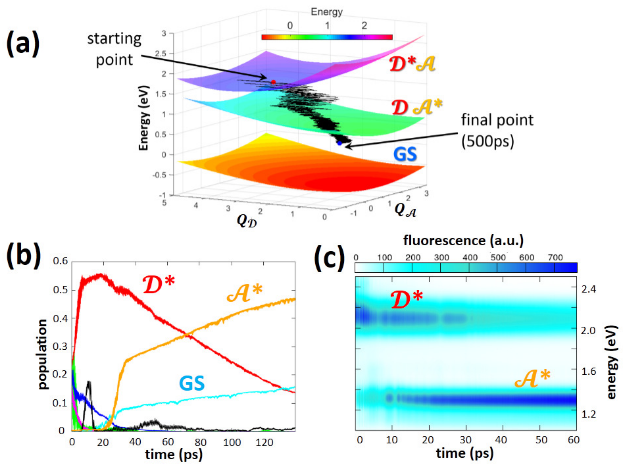

Figure 1: Resonance Energy Transfer in real time. (a) Non-adiabatic $\mathcal{D}\mathcal{A}$ dynamics following impulsive excitation of $\mathcal{D}$; to help the eye, relevant adiabatic potential energy surfaces (PES) are also shown. (b) Population time-dependence plotted for some relevant $\mathcal{D}\mathcal{A}$ states. (c) Time-dependent fluorescence spectra for the $\mathcal{D}\mathcal{A}$ system.

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# A New Route for the Determination of Protein Structure in Physiological Environment

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## Abstract

Revealing the structure of complex biological macromolecules, such as proteins, is an essential step for understanding the chemical mechanisms that determine the diversity of their functions. Synchrotron based x-ray crystallography and cryo-electron microscopy have made major contributions in determining thousands of protein structures even from micro-sized crystals. They suffer from some limitations that have not been overcome, such as radiation damage, the natural inability to crystallize of a number of proteins and experimental conditions for structure determination that are incompatible with the physiological environment. Today the ultrashort and ultra-bright pulses of X-ray free-electron lasers (XFELs) have made attainable the dream to determine protein structure before radiation damage starts to destroy the samples. However, the signal-to-noise ratio remains a great challenge to obtain usable diffraction patterns from a single protein molecule. We describe here a new methodology that should overcome the signal and protein crystallization limits. Using a multidisciplinary approach, we propose to create a 2D protein array with defined orientation attached on a self-assembled-monolayer. We develop a literature-based, flexible toolbox capable of assembling different proteins on a functionalized surface while keeping them under physiological conditions during the experiment, using a water-confining graphene cover.

# Photophysical behaviour of the binding of Cationic Al(III) phthalocyanines and Bovine Serum Albumin

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Metallophthalocyanines (MPcs), are second generation photosensitizers with intense absorption in the red region of visible light, selective localization in tumours and efficient generation of singlet oxygen, giving them their potential in photodynamic therapy (PDT) of cancer [1, 2]. Most drugs are transported by serum albumins in vertebrates [3], the interaction between drugs and protein could significantly affect the excretion and distribution of these drugs, and also affect their therapeutic activity and toxicity. Bovine serum albumin (BSA) shares properties of stability, water solubility, versatile binding capacity and structure homology (80%) with human serum albumin, and thus it is used as a model protein [4].

Photophysical and photochemical properties of quaternized water soluble AlPc peripherally and non-peripherally tetrasubstituted with N-methyl-2-pyridylthio group were studied in aqueous medium and in the presence of BSA. Large binding constant values, suggesting a strong interaction between BSA and the MPcs, was observed. Laser flash photolysis experiments revealed high triplet state quantum yields with corresponding long triplet state lifetimes which will result in high photosensitizing ability of the MPcs in the presence of BSA. The efficiency of singlet oxygen generation via energy transfer from the excited triplet state of the MPc to ground state oxygen increased markedly in the presence of BSA. Stern–Volmer quenching constant reveals static quenching as a probable mechanism of quenching of BSA fluorescence by the MPc.

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# Zero-waste, photo-induced functionalization of macroscopic carbon nanotube assemblies for flexible supercapacitors

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The physico-chemical properties of carbon nanotubes (CNTs) make them very interesting for many different applications (*e.g.* soft matter,[1] organ and nerve regeneration,[2,3] or catalysis[4]). To exploit the nanostructure properties on a macroscopic scale, they can be assembled into foams, films or fibers. Particularly, CNT fibers are especially attractive as their geometrical arrangement exploits the anisotropy of the building blocks. However, as-produced CNT fibers are highly hydrophobic preventing their utilization in applications where the interaction with water or polar solvents is required (*e.g.* sol-gel processes). Over the last decades, different routes have been developed to render hydrophilic the graphitic structure of CNTs. Most of these approaches are done under wet chemical conditions compromising the macroscopic structure of the fibers.

In this work, we have used UV-generated ozone to functionalize CNT fibers made of different precursors (*i.e.* butanol or toluene)[5]. The protocol appeared as a fast (*i.e.* 5 min to 2 h) and facile (*i.e.* no purification was required) way to functionalize the materials and increase their hydrophilicity with a very good control of the degree of functionalization, with generation of virtually zero-waste. All materials were characterized by Raman spectroscopy, transmission emission and scanning emission microscopy, X-ray photoelectron spectroscopy and we studied the effect of the functional groups in the mechanical and electrical properties of the assemblies. Eventually, we assembled flexible all-solid state supercapacitors with high energy density.

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# First step towards the description of hybrid organic-inorganic Nanosystems: simulating absorption spectra of gold nanoparticles with PCM approach

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Hybrid organic-inorganic Nanoparticles (HNPs) are very interesting and widely studied materials, for their versatile applications in biotechnology and medicine, with high potential in biomedical imaging, gene and drug delivery, and photothermal cancer therapy [1, 2], making them one of the most promising materials for early and accurate cancer diagnosis and effective cancer therapy. However, computing their physico-chemical properties in details proves to be a challenge. While the nature of the organic component of the HNPs necessitates a full quantum chemical treatment, the size of the inorganic component renders this treatment computationally too expensive to be assessed with an homogeneous technique.

For this reason hybrid models have been developed combining a QM level treatment and a classical electromagnetism approach, respectively, for molecules and the inorganic nano-structures upon which they are adsorbed [3]. In particular, the inorganic component, usually a metal, is considered as a continuous body, characterised by its own frequency dependent dielectric function (Polarizable Continuum Model, PCM), while excitation energies due to the energy transfer from the molecule to the metal is evaluated exploiting Time Dependent Density Functional Theory (TDDFT).

The first step towards a correct application of this model is to prove that the polarization charges distribution, introduced by PCM, well describes the optical properties of bare inorganic Nanoparticles. With this scope, experimental spectra [4, 5] of bare gold Nanoparticles have been reproduced using PCM tools.

Future steps will evaluate the organic molecular frame at quantum chemical level and describe its interaction with the Nanoparticles in order to reproduce the desired spectroscopical properties for the hybrid system.

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# Two-photon anisotropy: experiments and models

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## Abstract

Optical spectroscopy is a powerful tool to investigate structure-properties relationship in molecular systems, addressing not only ground state but excited states properties as well. Non-linear spectroscopy plays a fundamental role, since it allows to investigate states which are not active in linear processes. In particular two-photon anisotropy allows to obtain extremely detailed information about the relative orientation of transition dipole moments involving high excited states. To fully exploit this potential we need interpretative tools, i.e. theoretical models.

This work focuses on multipolar organic dyes, and exploits the approach of essential states model. Experimental spectra of two-photon anisotropy have been compared with results from essential states models. Observed anisotropy spectra sharply contrast with the expectations based on simple symmetry arguments, but can be rationalized quantitatively, if the coupling of electronic motion to molecular vibrations and polar solvation is properly accounted for. Here we present for the first time a complete calculation of two-photon induced anisotropies, also addressing bandshapes, based on models that were developed and parametrized to reproduce other spectral properties.

# LIGHT INTERACTIONS ON CORN SEED GROWTH UNDER SIMULATED MICROGRAVITY

**Conference on the Complex Interactions of Light and Biological Matter: Experiments meet Theory (smr 3120), 21-25 May 2018**
**International Centre for Theoretical Physics (ICTP), Trieste, Italy.**

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## INTRODUCTION

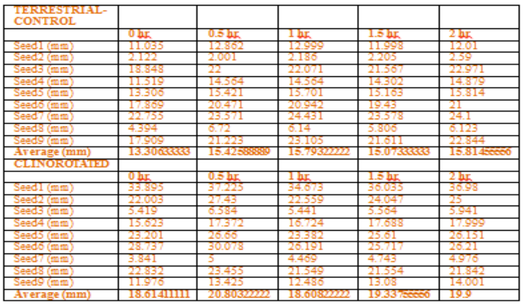
Living organisms are made-up of cells. Cells on the other hand are made-up of several macromolecules such as proteins, carbohydrates, nucleic-acids, lipids etc which have individual functions. The role and impact of light on plant metabolism including photosynthesis cannot be overemphasized. Corn (*Zea mays*) is an important grain used for food, animal fodder, the production of alcoholic beverages, and biofuels. Experimental sample of corn-seeds were allowed to grow under simulated microgravity using clinostat for 4hours. The experimental and the control samples had equal treatment by receiving 50lux of light and humidity of 60-100%. These are essential for photosynthesis. Observations and analysis were done using ImageJ software on the pictures taken periodically on the two samples for the period of the four hours. Haven received equal light treatment, the quantitative analytical result on the growth gives information on the light interactions on the individual samples from their photosynthesis.

## METHODOLOGY

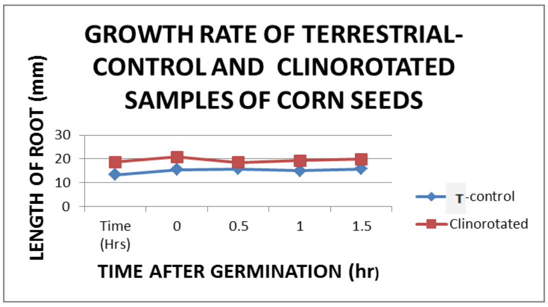
The substrate of seeds called plant-agar was prepared into 2petri-dishes following the standard preparation method. Then the corn-seeds were planted into the substrate and it was cultivated inside a wet chamber in vertical positions. After 3 days, germination of the seeds with short roots was observed. The 2petri-dishes were then taken and labeled "terrestrial-control", and "clinorotated". The terrestrial-control sample was remained in the vertical position while the clinorotated sample was placed at the centre of the clinostat using double-sided tape. The photos of the 2petri-dishes were taken every 30minutes with very short stopping time of the clinorotated in order to avoid the effect of gravity. These observation was done for 4hr under the following conditions. Light of 50lux (measured using lux metre), humidity between 60% to 100% and temperature of 23°C. In addition to these, the clinorotated sample had the following conditions, rotation speed of 75rpm, horizontal rotational-axis angle of 90° and the direction of rotation was clockwise. At the end of observation, the analysis of growth-rates were carried out. The data obtained were the two sets of photos of the roots which show the "terrestrial-control" and "clinorotated" roots. An image-processing application soft-ware called ImageJ was used to analyse these photos. The difference between the two cases was analyzed by measuring the length of the roots, which thereby allowed their growth-rate to be determined. This was done by using the length measurement tool and measuring a fixed length in the photo. This yielded data-set of experimental-results in gravity and simulated microgravity responses whose grand average was calculated in mm/hr and used to plot graph (United Nations, 2013).

## RESULT

The average growth-rate of the roots for the terrestrial-control sample was 7.54mm/hr while that of the clinorotated sample was 9.73mm/hr. The table below shows the growth-rate analysis using the root length of the terrestrial-control and clinorotated samples while the graph was plotted using the averages from the table.



| TERRESTRIAL-CONTROL | | | | | |
|---|---|---|---|---|---|
| | 0 hr | 0.5 hr | 1 hr | 1.5 hr | 2 hr |
| Seed1 (mm) | 11.035 | 12.862 | 12.999 | 11.998 | 12.01 |
| Seed2 (mm) | 2.122 | 2.001 | 2.186 | 2.205 | 2.59 |
| Seed3 (mm) | 18.848 | 22 | 22.071 | 21.567 | 22.971 |
| Seed4 (mm) | 11.519 | 14.564 | 14.564 | 14.302 | 14.879 |
| Seed5 (mm) | 13.306 | 15.421 | 15.701 | 15.163 | 15.814 |
| Seed6 (mm) | 17.869 | 20.471 | 20.942 | 19.43 | 21 |
| Seed7 (mm) | 22.755 | 23.571 | 24.431 | 23.578 | 24.1 |
| Seed8 (mm) | 4.394 | 6.72 | 6.14 | 5.806 | 6.123 |
| Seed9 (mm) | 17.909 | 21.223 | 23.105 | 21.611 | 22.844 |
| Average (mm) | 13.30633333 | 15.42588889 | 15.79322222 | 15.07333333 | 15.81455556 |
| CLINOROTATED | | | | | |
| | 0 hr | 0.5 hr | 1 hr | 1.5 hr | 2 hr |
| Seed1 (mm) | 33.895 | 37.225 | 34.673 | 36.035 | 36.98 |
| Seed2 (mm) | 22.003 | 27.43 | 22.559 | 24.047 | 25 |
| Seed3 (mm) | 5.419 | 6.584 | 5.441 | 5.564 | 5.941 |
| Seed4 (mm) | 15.623 | 17.372 | 16.724 | 17.688 | 17.999 |
| Seed5 (mm) | 23.201 | 26.66 | 23.382 | 25.61 | 26.151 |
| Seed6 (mm) | 28.737 | 30.078 | 26.191 | 25.717 | 26.21 |
| Seed7 (mm) | 3.841 | 5 | 4.469 | 4.743 | 4.976 |
| Seed8 (mm) | 22.832 | 23.455 | 21.549 | 21.554 | 21.842 |
| Seed9 (mm) | 11.976 | 13.425 | 12.486 | 13.08 | 14.001 |
| Average (mm) | 18.61411111 | 20.80322222 | 18.60822222 | 19.33755556 | 19.9 |



## DISCUSSION AND CONCLUSION

The quantitative result of the average growth-rate of the roots of the corn indicated an increased growth-rate of corn under simulated microgravity by 28.97%. The two samples received equal lux of light, but the interaction of the light for conversion into chemical-energy for plant activities was different after subjection to simulated-microgravity for 4hours. It could be deduced that: the light dependent reactions, which takes place in the thylakoid membrane, that use light energy to make ATP (chemical) and NADPH was speed-up under simulated-microgravity and that photosynthetic functions are affected by the space environment (Howard, 2010). Therefore, role of light on plants is complex and this is a function of the role of complex light interactions on individual cells of the plant.

## ACKNOWLEDGEMENT

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# Heterochiral tripeptides nanostructures

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## Abstract

In the last two decades, nanoscience has grown esponentially, obtaining several kind of materials for many applications, in particular for drug delivery systems. Hydrogel class has been investigated and it was proposed that low-molecular weight peptide-based hydrogelators (LMWGs) could be used as safe biomaterials. The innovative use of D-amino acids in combination with L-amino acids to create new self-assembling tripeptides materials able to create a well-organized supermolecular structure suitable for medical applications. The nanostructures of these materials could be characterized using different kind of spectroscopic techniques, i.e. infrared spectroscopy or circular dichroism spectroscopy to help to understand better the behaviour of these ultra-short peptides, since usually more informations are available for bigger and more complex peptides and proteins.

# Visible light reverts the effect in motility produced by temperature in mouse sperm

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## Abstract

The effects of visible light on biological systems have been studied for several years, from mammal spermatozoa motility to protein structural changes. The data have shown that these systems interact in certain ways with light but the origin and mechanisms are still far from being understood. Thus more work on the subject is needed. In the present work we study the effects of green light (490-540 nm) on the motility of mouse spermatozoa with an optical technique of time-resolved correlation adapted to study several samples simultaneously. Image correlation analysis is used to follow the temporal behavior of the sperm samples at 10 ºC and 37 ºC . At these contrasting temperatures, the motility is radically different: at the lower one the prevalence is the lengthiest, according to a previous finding reported by us. Our present results show that while green light extends the prevalence of sperm motility at 37 ºC, it reduces it at 10 ºC. This evidence suggests that green light is playing an important role in the spermatozoa motility. Also, Atomic Force Microscopy measurements were made to detect changes in the mechanical properties (adhesion forces) of the spermatozoa under the effect of green light. We speculate about the possibility that these opposed effects are related to elastic changes that spermatozoa suffer during irradiation.

# Understanding Metal Induced Color Expression in Anthocyanins

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## Abstract

Use of artificial colorants in the food industry has declined due to health concerns and consumer demand, increasing the popularity of natural alternatives. Anthocyanins are a class of naturally occurring pigments that produce red-purple-blue in nature, especially when interacting with metal ions. Recently, experiments show that many metal ions have been found to induce bathochromic shifts on the visible absorption spectra of anthocyanins. We present one of the first theoretical studies to evaluate the effects of metals on the absorption spectra of anthocyanins. In this work we have adopted the multi scale computational method developed in our group to study how the presence of metal ions affect the geometry of anthocyanins, directly linked to the absorption spectra. We have also examined how the electronic structure is modified due to the presence of metal ions. Furthermore, we have investigated different ratios between anthocyanin and metal ions.

# Repurposing of FDA approved drugs reveals novel Hsp90 inhibitors: A structure-based drug design study.

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Molecular chaprone Heat Shock Protein 90 (Hsp90) represents an interesting chemotherapeutic target for cancer treatments, as it play role in cancer proliferation. This work aimed to identify novel Hsp90 inhibitors as anticancer agents. Repurposing of FDA approved drugs was carried out using a relaxed complex scheme an *in silico* method. FDA approved drugs were screened from DrugBank data base. Two drugs; 5-4-[4-(5-cyano-1H-indol-3-yl)butyl]piperazin-1-yl-1-benzofuran-2-carboxamide known as vilazodone and (3R,4S)-1-(4-fluorophenyl)-3-[(3S)-3-(4-fluorophenyl)-3-hydroxypropyl]-4-(4-hydroxyphenyl)azetidin-2-one known as ezetimibe were identified as novel potent inhibitors of Hsp90$\beta$. Docking and molecular dynamic studies of these drugs revealed a second binding pocket. Vilazodone showed strong binding in the second pocket suggesting it to be an allosteric inhibitor. The role of water on Hsp90-drug interaction was investigated. Water was observed to mediate the interaction of some drugs with Hsp90. However, in some cases, water did not mediate the interaction between Hsp90-drugs complex. The identified drugs are further recommended for pre-clinical and clinical evaluation. The study also recommends on the sensitivity of the relaxed complex scheme and the inclusion of water during molecular docking.

# Intrinsic fluorescence properties of single amino acids

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## Abstract

Amyloid fibrils, associated with diseases such as Alzheimer's and Parkinson's, display an intrinsic fluorescence in the visible range. This intrinsic fluorescence is present in structures devoid of aromatic residues. Investigation into this phenomenon showed that the observed fluorescence is related to proton delocalisation in short hydrogen bonds [1].
To investigate the origin of this intrinsic fluorescence further we studied the optical properties of single amino acids, L-glutamine, L-lysine and L-alanine. Upon incubation of various amino acids in H2O at 65°C, each amino acid displayed different optical properties upon incubation. L-alanine becomes fluorescent upon initial addition of H2O, L-lysine also becomes fluorescent upon addition of H2O, but decreases in fluorescence over time. L-glutamine is not florescent upon addition of H2O but increases in fluorescence over time. All samples had similar excitation and emission peaks, at ~360 nm and 430 nm, respectively. X-ray diffraction of dried L-glutamine after 4 days incubation at 65°C shows that a new structure is forming which is similar to pyro-L-glutamine but containing an associated ammonium ion. Short hydrogen bonds forming between the newly formed pyro-L-glutamine and the ammonium ion give rise to the intrinsic fluorescence observed. Further investigation into the properties of L-lysine and L-alanine fluorescence using MD simulations will provide more information about the intrinsic fluorescence observed in proteins.

# Effect of Aryl Substitution on the Chiroptical Properties of Supramolecular Assemblies

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Chiral groups on molecular systems have an important influence on the organization of molecules of helical arrangements. The effect of the multiple transition dipole moment on the single molecular system on the chiral features of supramolecular assembly has been less understood. To investigate these aspects, we have designed four chiral molecular systems having D- and L-isomers of phenylalanine, functionalized onto the meta-position of the terminal phenyl groups of two sets of phenyleneethynylenes: (a) 1,4-bis(phenylethynyl)-2,5-bis(dodecyloxy)benzene and (b) 1,4-bis (phenylethynyl)-2,5-bis(dodecyl)benzene. In the present case, the effect of dialkoxy group on the circular dichroic properties is investigated by replacing dodecyloxy groups in the central phenyl ring of former set of molecules by dodecyl groups. By adopting various spectroscopic methods, we explore the asymmetric organization of these molecular systems and the role of various transition dipoles on the origin of chiroptical properties. These aspects are rationalized in terms of a simple and computationally cost-effective semiempirical bottom-up methodology, based on a generalized exciton model.

1. James, P. V., Sudeep, P. K., Suresh, C. H., Thomas, K. G., *J. Phys. Chem. A* **110**, 4329 (2006).

# Superlinear amplification of the first hyperpolarizability of linear aggregates of DANS molecules

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## Abstract

A bottom-up modelling strategy is adopted to discuss the linear and nonlinear optical spectra of a prototypical push-pull dye, 4-dimethylamino-4′-nitrostilbene (DANS), in different environments, from solutions to linear aggregates, fully accounting for the molecular polarity and polarizability. In particular, we demonstrate a large amplification of the first hyperpolarizability of linear aggregates with a superlinear dependence on the aggregate size. Results are discussed with reference to recent experiments for DANS molecules aligned inside single-wall carbon nanotubes, leading to a complete and internally consistent description of the observed spectral properties in terms of ~7 aligned molecules, reducing by an order of magnitude the size of the aggregate estimated in the hypothesis of linear amplification, as expected for non-interacting molecules. This has important implications for material design: it is possible to obtain a large amplification of the first hyperpolarizability by aligning just a few DANS molecules (or more generally, a few polar dyes showing normal solvatochromism) without the need to grow large ordered systems.

# Time- Dependent Fluorescence Stokes Shift of Monellin

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## Abstract

Monellin being potent sweet in nature finds the application in substituting the high-calorie sugar derivatives and get rid of artificial sweeteners: the commercially preferable form still being the subject of research to overcome the low-temperature denaturation. The time-resolved fluorescence phenomenon in this complex protein helps in understanding the various time scales involved in the solvation process which further helps in understanding the several features of protein in general. Such time scale clearly indicates the processes involved in the formation of the structure and provides us with an elementary understanding of the protein folding though being in the naive sense. The method further can be utilized to find the synchronizing pattern among the various other sweet protein which is currently lacking. The molecular dynamics study reflects the time-scales of femtoseconds to tens of picoseconds are the prominent one and each scale correspond to of freedom associated with the structures. The research can be used to understand the importance of Statistical Mechanics in predicting the behaviour of the biomaterials.