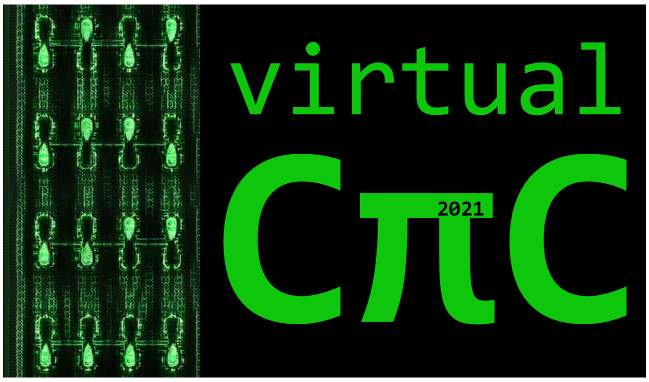
12th European Symposium on

Computing π-conjugated Compounds



18th January - 20th January 2021
Virtual Edition

Book of Abstracts

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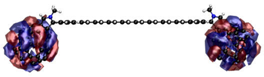

Welcome to first virtual CπC!

Dear Friends and Colleagues,

we are pleased to welcome you to the *12th edition of the Symposium on Computing π-conjugated Compounds*. For those who are not familiar with CπC, this is a series of symposia that offers an informal forum for the discussion of the latest advances in the theoretical and computational research on pi-conjugated systems.

The unfortunate situation due to the pandemic outbreak, lead us to switch to an different format for this 2021 edition. We are all aware of the importance of the social dimension of this symposium and how hard it will be to provide it through an online interface - nevertheless we thought it would have been a mistake to skip 1-year and decided to organize a virtual edition of the CπC (virtual CπC), as an online event held on 18th - 20th January 2021.

We still hope to offer you a great opportunity for a fruitful and open scientific exchange - hopefully the same that characterized the previous editions of CπC. We will do our best to keep it as smooth as possible, facilitate discussions after oral presentations and during the poster session. More detailed indications on how to participate are indicated in the following page.

The CπC spirit is always the same, even though some exceptional reshaping turned out to be necessary for this edition:

Keep it small! This edition attains almost 100 participants, doubling the typical size of CπC meetings. This is certainly the result of the online format, but it also reflects the enthusiastic response from our community!

Keep it cheap! Can you imagine a symposium cheaper than this one?

Think local! In an online conference, planet earth is the limit! We are hence delighted to host renewed invited speakers we would not have the occasion to listen to in an ordinary edition.

Widen the horizon! Get ready to take up a great “experimental challenge” on coherent phenomena in chemical reactions.

Think young! All contributed talks will be from early-stage researchers. This is our response to the lack of opportunities that students and postdocs are facing during this global crisis.

Discuss it! The interesting part of a talk begins after its end. A discussion in front of a poster may give enlightening inputs to your research. Enjoy the virtual CπC room on Wonder! This is the place to meet, discuss, and maybe envision a beautiful collaboration.

The Organization Board of the 12th Symposium on Computing π-conjugated Compounds

Gabriele D’Avino, Luca Grisanti, Mathieu Linares, Giacomo Prampolini

VIRTUAL CπC INSTRUCTIONS

The oral sessions will take place on `Zoom`, the poster session will be on the `Wonder` platform. **The links and the instructions to connect will be emailed on Monday morning.**

For the good success of the online Symposium, we kindly ask all participants to adhere to the following recommendations:

- Make sure you are equipped with an adequate computer, a `Zoom` client installed and tested,
- A browser up-to-date (someone reported compatibility problems with some version of Safari browser), a microphone, and stable internet connection. The use of a camera would be greatly appreciated for the speakers.
- All participants can connect with microphone and camera. You might be asked to switch your camera off in case of connection issues.
- Questions to the speakers and contributions to the discussion should be typed in the public chat.

ENJOY THIS VIRTUAL CπC!

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15:10	15:30	**P2**	**D2**	**O2**
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2	Silvio Osella
3	Irene Casademont Reig
4	Daniel Aranda Ruiz
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6	Stefan Knippenberg
7	Alexandra Harbuzaru
8	Sergio Gámez Valenzuela
9	Yogesh Todarwal
10	Otello M Roscioni
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19	Dang Khoa Andrea Phan Huu

Invited oral presentations

Excitons and Polarons in Organic Materials

Frank C. Spano,*[a] Raja Ghosh[a]

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Excitons and polarons play a critical role in the electronic and optical properties of aggregates, thin films and crystals of π-conjugated molecules and polymers. In such systems neutral excitations (excitons) and charged excitations (polarons) are coupled strongly to nuclear degrees of freedom involving the symmetric vinyl-stretching mode (i.e. the aromatic-quinoidal vibration when conjugated rings are present). In this talk the photophysical properties of excitons and polarons in organic materials are compared and contrasted within the framework of the Holstein Hamiltonian, which treats electronic coupling and local electron-vibrational coupling on equal footing.[1] Applications are made to excitons and positively-changed polarons (holes) in poly(3-hexylthiophene) films.[2, 3] It is shown how simple optical probes can be used to extract the exciton and polaron coherence lengths, quantities which are important for understanding energy and charge transport.

References

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Coherence in reactions

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I will discuss coherence phenomena as a probe of electron transfer (ET) reactions. Vibrations enable a dramatic speed up for some ET reactions, or control of ET by suppressing and enhancing reaction paths. Despite these, and other, compelling examples of the function of vibrations in ET reactions, experimental resolution of the mechanism of interplay of ET with vibrations has eluded researchers. Here I report ultrafast coherence experiments that resolve how quantum vibrations participate during an ET reaction. We observe generation—by the ET reaction, not the laser pulse—of a new coherence along a reaction coordinate in a mode associated with the reaction product. This surprising spontaneous launch of a vibrational wavepacket shows that coherence can be generated by a separation of timescales in chemical dynamics, and not solely by pulsed laser photoexcitation.

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Molecular Spectroscopy in Condensed Phases: the Medium Polarizability

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Electrostatic intermolecular interactions are responsible in molecular materials for several intriguing phenomena, including exciton delocalization and energy transfer. In these two examples, each molecule interacts with nearby molecules, with overlapping, or almost so, spectral features. Molecules in solution instead interact with a medium that, by choice, is transparent in the spectral region of interest, yet important solvation effects are recognized in optical spectra. The different timescale of the molecular degrees of freedom vs the solvent degrees of freedom is the key to all effective solvation models that rely on the definition of a molecular Hamiltonian, renormalized to account for the interaction with the solvent. All available effective solvation models, where the solvent is described as a continuum dielectric medium (PCM, COSMO, etc) or at the atomistic detail (like e.g. in QM-MM approaches) rely on the adiabatic approximation to disentangle solvent and solute degrees of freedom. In the adiabatic approximation, a molecular Hamiltonian is defined for the solute experiencing the electrostatic potential generated by the solvent in a fixed configuration, typically corresponding to the equilibrium configuration for a specific state of the solute. The adiabatic approximation is certainly reliable to disentangle the slow degrees of freedom of the solvent, related to polar solvation, but it is physically untenable when applied to describe the effects of the electronic polarizability of the solvent on molecular properties and spectra. The electronic polarizability of the solvent in fact related to electronic solvent excitations typically located far in the UV. An antiadiabatic separation of the motions is therefore needed to properly address the effects of the medium polarizability (as measured e.g. by the solvent refractive index) on molecular properties and spectra [1]. In this approximation, a single effective molecular Hamiltonian is defined, where the solvent polarizability enters as a two-electron term, that, in the dipolar approximation, is simply proportional to the squared molecular dipole moment. To illustrate this point, we will shortly discuss the pitfalls of current implementations of continuum solvation models in popular computational packages, comparing relevant results with those obtained in the antiadiabatic approximation. [2]

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Contributed oral presentations

Bidimensional H-Bond Network Promotes Structural Order and Electron Transport in Pyridyl-Based Molecular Semiconductors: A Computational Study

Andrea Giunchi,*[a] **Luca Muccioli,**[a] **Gabriele D'Avino,**[b] **Antonio De Nicola,** [c] **Andrea Correa,** [d] **Junji Kido,** [c] **Giuseppe Milano** [c,e]

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b) Grenoble Alpes University, CNRS, Grenoble INP, Institut Néel, France
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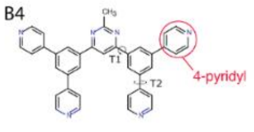
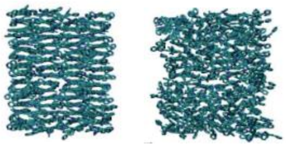
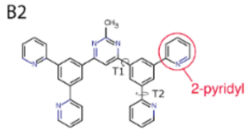
The two electron-transporting molecular semiconductors B2 and B4 (4,6-bis(3,5-di(pyridine-n-yl)phenyl)-2-methylpyrimidine with n = 2 or 4, respectively) represent a puzzling and relevant case study in organic electronics. While these two molecules differ only for the position of N atoms in terminal pyridine groups, their thin films show remarkable differences in molecular organization and, most importantly, in the electron mobility that is 2 orders of magnitude higher in B4 than in B2.[1]

In this study[2] we combine MD, DFT and ME calculations to unravel the microscopic origin of structure-property relationships in B2 and B4, with the ultimate goal to better understand factors that can promote structural organization and good charge transport properties, such as Van der Waal interactions in molecular films.

We found that B4 has a higher capability to connect with adjacent molecules by intermolecular hydrogen bonds, compared with B2. The stronger 2D H-bond network formed for B4 is sufficient to stabilize a supramolecular organization in which molecules form ordered layers and columns. The calculation of essential electron transport parameters, such as reorganization energies, site energies, and electronic couplings revealed that the microscopic origin of the higher electron mobility of B4 with respect to B2 has its roots in lower reorganization energy and electrostatic disorder and, more importantly, in the superior morphology promoted by the hydrogen bond network. On a general vein, our findings disclose how intermolecular hydrogen bond interactions promote structural order in molecular thin films, ultimately improving their electron transport properties. The engineering of these weak interactions offers viable opportunities for the rational design of new materials with improved performances in OLED applications.







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Collective screening phenomena prompt free-carrier release in doped organic semiconductors

Massimiliano Comin,*[a] Simone Fratini,[a] Xavier Blase,[a] Gabriele D'Avino,[a]

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The success of electronic and optoelectronic technologies relies on the possibility to tweak the energies of transport levels by molecular doping. In this context, Coulomb interactions between host molecules and ionized dopants play a key role in the energetics of doped organic semiconductors as they control dopant ionization, but also lead to strongly bound charge carriers. [1,2] By taking the paradigmatic case of F4TCNQ-doped pentacene, we show with first-principles calculations that the charge-transfer polarizability associated with host-dopant complexes can be up to one order of magnitude higher than that of the host semiconductor. The consequence of this dopant-induced increased polarizability is a dramatic enhancement of the macroscopic dielectric response of the doped material, ultimately helping the release of free carriers. Classical Micro-Electrostatics calculations reveal that the bulk dielectric response of the doped semiconductor tends towards a divergence at doping concentrations of 5-7%, similar to those determining conductivity enhancements of a few orders of magnitude in typical experiments. Our results suggest that such a doping-induced dielectric catastrophe may represent a driving factor for the insulator-to-metal transition in doped organic semiconductors. [3]

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Water Intake and Ion Exchange in PEDOT:Tos Film upon Cyclic Voltammetry: Experimental and Molecular Dynamics Investigation

Najmeh Delavari,*[a] Johannes Gladisch,[a] Ioannis Petsagkourakis,[a] Mohsen Modarresi,[b] Eleni Stavrinidou,[a] Mathieu Linares,[a,b,c] Igor Zozoulenko[a]

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Conductive polymer PEDOT:Tos (3,4- ethylenedioxythiophene doped with molecular tosylate) gained a considerable attention in various devices for bioelectronic applications, such as organic transistors and sensors. Many of these devices function upon oxidation/reduction processes in contact with aqueous electrolytes. So far, a theoretical insight into morphological changes, ion injection and water intake during these processes was rather limited. In the present work, we combined experiment and molecular dynamics simulations to study the water intake, swelling and exchange of ions in PEDOT:Tos film during the cyclic voltammetry. We showed that the film underwent significant changes in morphology and mass during the redox processes. We observed both experimentally and in simulations that the film lost its mass during reduction as tosylate and Na was expelled and gained mass during oxidation mainly due to the uptake of anions, i.e. tosylate and Cl. The relative mass change between the most oxidized and reduced states was ~10-14% according to both experiment and simulations. We detected an overall material loss of the film during voltammetry cycles indicating that a portion of the material leaving the film during reduction did not return to the film during the consecutive oxidation. Our combined experimental/simulation study unravelled the underlying molecular processes in the PEDOT:Tos film upon the redox process, providing the essential understanding needed to improve and assess the performance of bioelectronic devices.

Aromaticity of Excited Conjugated Rings: Baird or Hückel?

Silvia Escayola[a,b]*, **Claire Tonnelé**[b], **Eduard Matito**[b,c], **Albert Poater**[a], **Henrik Ottosson**[d], **Miquel Solà**[a], **David Casanova**[b,c]

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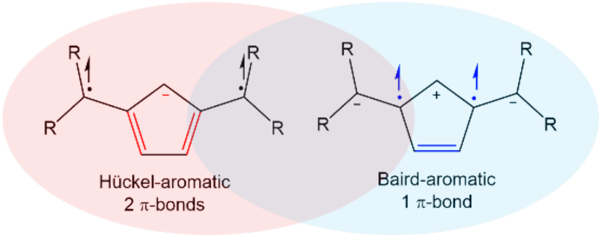
The increasing interest in systems with excited state aromaticity requires comprehensive and critical analyses combined with solid computational assessments for the proper interpretation of experimental data. Especially, since there is currently no spectroscopic technique that can be used as the sole method to evaluate this phenomenon. Here we are interested on characterizing the excited state aromaticity of TMTQ (an oligomer composed of a central 1,6-methano[10]annulene, and two 5-diacyanomethyl-thiophene exocyclic groups) and a series of other symmetrically substituted conjugated rings. The particular case of TMTQ, seems to generate controversy in the interpretation of the results. Even though, the low-lying excited states were theoretically characterized as Hückel-Baird hybrids, with a ca. 85% of Hückel and 15% of Baird character[1], a recent experimental study claimed that the S_1 is stabilized by Baird aromaticity[2]. In light of the new existing experimental data, we decided to reinvestigate the problem using (time-dependent) density functional theory methods. Our results showed that the interpretation by D. Kim and coworkers needs to be revised because the low-lying excitations of symmetrically substituted conjugated rings including TMTQ hold very weak charge transfer character. We also found that the high Baird character of the central ring is achieved only with anionic and small conjugated central rings with electron donating groups as substituents and small exocyclic groups with electron withdrawing substituents. Our study aims to warn about the need to make correct interpretations of the experiments in this area of research, as only then can the excited state aromaticity concept be developed into a useful tool for the design of high-performance organic electronic devices.



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Manipulating photochemistry under strong coupling to confined light modes

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Recent experiments have shown that the interaction between molecular transitions and confined light modes hosted in optical cavities can be exploited to manipulate chemical phenomena in the strong coupling regime [1-3]. When the interaction rate between a molecular transition and a cavity mode is faster than their intrinsic decay processes, the system enters the strong coupling regime and new hybrid light-matter states known as polaritons are formed. Although strong coupling between cavity modes and atoms or inorganic semiconductors has been extensively investigated in the context of condensed matter physics and quantum optics, the potential to manipulate chemical phenomena has only recently been explored. This has lead to the birth of polaritonic chemistry [4-7], an emerging field aiming to manipulate chemical dynamics and material properties through the formation of polaritons.

An important aspect of strong coupling is that it is a collective effect, meaning that an ensemble of molecules interacts with a confined light, and therefore, the polariton excitation is shared amongst all the molecules under strong coupling. In the collective situation, additional dark states are also present as opposed to the single-molecule case. These dark states are superpositions of all the molecular excitations of the ensemble and are uncoupled from the confined light mode. Given that experimental realisations of electronic strong coupling involve a macroscopic number of molecules, the role played by the dark states in the nonadiabatic dynamics should be understood.

In this talk I will introduce electronic strong coupling with organic molecules and I will focus on a photoisomerization example that highlights the importance of disorder in the composition of polaritons and dark states, with important consequences on the excited-state relaxation and photoisomerization efficiency. I will also discuss the usefulness of polaritonic potential energy surfaces [8] to gain insight on photochemistry under electronic strong coupling.

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Frustrated magnetism in a cyclacene crystal

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We consider a triangular lattice of short carbon nanorings (cyclacenes). In the single molecule limit, each unit has 2 topologically protected zero modes. As a result, we could expect the low energy bands of the cyclacene crystal to be formed by the zero modes and realize two coupled triangular lattices of zero modes. When Coulomb repulsion is added into this picture, the low energy physics of this system should be similar to a Hubbard model of two weakly coupled triangular lattices. In the strong coupling limit, every ring should host 2 localized electrons, correlated antiferromagnetically with each other, and with the first neighbour ciclacene's, producing antiferromagnetically coupled frustrated S=1/2 triangular lattices. We carry out DFT calculations that confirm the main features of this scenario and show a non-collinear 120 antiferromagnetic phase ground state. Our results show a bottom-up route to engineer correlated electronic phases with narrow bands in carbon-based crystals, complementary to the top-bottom twisted bilayer approach.

Controlling the Extent of Diradical Character in Dicyanomethylene-substituted Indolocarbazoles

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Recently, dynamic covalent bonds receive lot of attention because of their unique feature to become reversible under mild conditions.[1] Interestingly, π–conjugated diradical compounds have emerged as essential building blocks in DCC (dynamic covalent chemistry).[2] We have recently demonstrated the potential of carbazole units substituted with terminal dicyanomethylene (DCM) groups to act as building blocks in DCC.[3] However, until now, the analysis of the dynamic covalent properties in indolocarbazole-based systems has not been approached. In this work, we investigate for the first time how the elongation of the conjugated core and molecular isomerism in indolcarbazole diradicals impact on the self-assembly formation of the resulting stimuli-responsive cyclophanes.[4] Among other interesting results, we demonstrate that an indolo[3,2-b]carbazole containing terminal dicyanomethylene groups, ICz-CN (see figure 1), is able to form a σ-dimer structure with two co-facial indolocarbazole units showing a strong strong chromism from light yellow to blue-green upon bond dissociation.

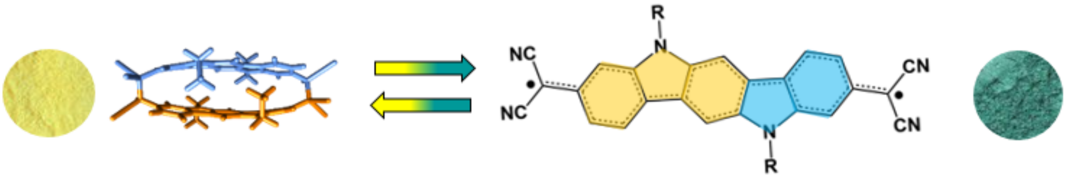

Figure 1. Equilibrium between an isolated ICz-CN and its corresponding σ-aggregate structure.

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Quantum dynamics of ultrafast decay of the excited states of Cytosine and its derivatives in the gas phase based on TD-DFT and LVC Hamiltonians

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The rapid excited state relaxation of isolated DNA bases (Adenine, Cytosine, Thymine, and Guanine) make them highly stable against UV irradiation.[1] On the other hand, modified DNA bases, especially 5-methylcytosine play vital roles in the epigenetic control of gene expression.[2] Investigation of the photochemical and photophysical processes in isolated bases can help to unravel their remarkable self-protection against photodamage. Although in the last decade a large number of theoretical and experimental studies have been devoted to elucidate the excited state dynamics, a full understanding of the photophysics of DNA bases and their derivative is still lacking.[3] Computational and experimental studies confirm that despite the crucial direct relaxation of the bright excited states to ground state, ππ*/nπ* internal conversion is also involved in the decay process of cytosine, cytidine, and 5-methylcytidine.[4] Most computational studies so far have investigated the excited state dynamics of nucleobases with semiclassical approaches. In relation to this, herein we investigate the ultrafast ππ*/nπ* decay of cytosine and its derivatives in the gas-phase with a full quantum dynamical (QD) calculation.

In this study, we used 1-methyl-cytosine and 1,5di-methylcytosine as a model for cytidine and 5-methyl-cytidine respectively, and performed QD simulations based on a Linear Vibronic Coupling (LVC) Hamiltonian. The LVC Hamiltonian is parameterized with TD-DFT adopting two different functionals, CAM-B3LYP and PBE0 and the 6-31+G(d,p) basis set. The purpose of our study is to investigate the effects of substituents and excitation wavelength on the decay process. To that end, we parametrized our LVC Hamiltonians at different points (Franck Condon (FC) point and excited states minima). Moreover, we analyse the nuclear dynamics associated with the time evolution of the excited states decay. Almost all calculations predict for initial photo-excitation on the first two bright states, a fraction of the population flows into nπ* states. From quantitive point of view, we observed that our results are sensitive on the energy gap between ππ* and the nπ* states, which depends on the functionals adopted to parametrize the LVC Hamiltonian.

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Dual classical/quantum MD strategy for the determination of site energies in photosynthetic complexes: Application to the PC645 antenna

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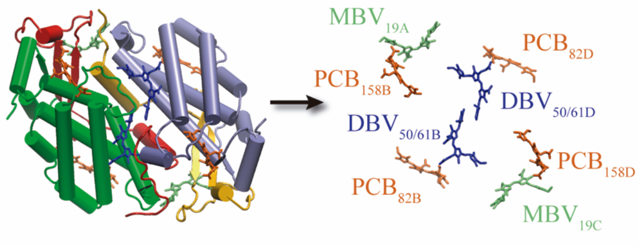
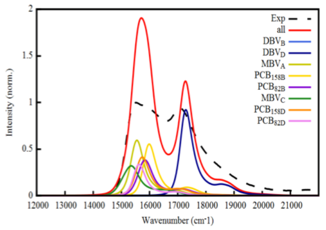
The light-harvesting mechanisms of photosynthesis are the focus of intense research due to the desire to mimic their efficiency in artificial devices. In the last decade, advances in 2D electronic spectroscopy has revealed unprecedented details, for example, in the energy transfer processes occurring in photosynthetic antenna complexes, like the observation of quantum beatings that seem to imply a role of coherence in the transfer.[1] The development of quantitative models of light-harvesting able to rationalize spectroscopic observations rely however on our ability to determine with sufficient accuracy key parameters controlling exciton dynamics, like pigment site energies.[2] In this study, we apply a dual molecular dynamics (MD) multiscale strategy to determine the site energies of the PC645 antenna complex from cryptophyte algae.[3,4] The strategy combines classical MD simulations on the ms timescale, with multiple short Born-Oppenheimer QM/MM MD simulations on the ps timescale, which allow to accurately describe pigment's vibrations. The structures are then used to evaluate pigments excited states using advanced polarizable QM/MM (MMPol) calculations performed at the TD-DFT level.[2,5] We show that this strategy significantly improves protocols based on either classical MD or single QM/MM optimizations of the pigments in the protein scaffold, and paves the way for an accurate determination of not only site energies, but also dynamic and static disorder effects, which play an important role in energy transfer dynamics.





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Understanding Förster energy transfer through the lens of molecular dynamics

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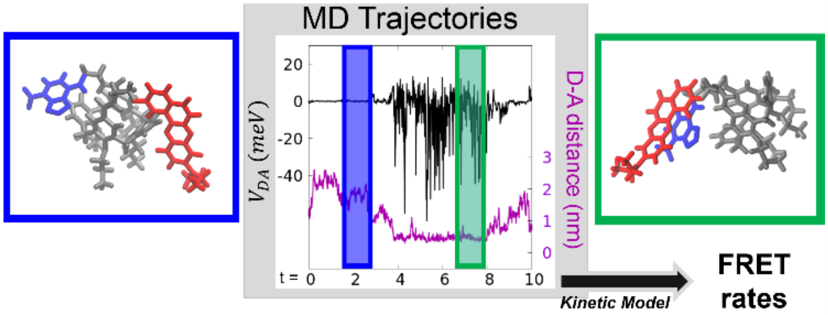
Resonance energy transfer (RET) describes a process where energy is transferred from an excited molecule, called the energy donor (D), to an acceptor molecule (A). RET plays a major role in nature, where among other things, it governs the physics of photosynthesis, taking part in the very first steps of the process. RET finds extensive applications in optoelectronic devices, bioimaging, and bioanalysis. In this research we investigate Förster RET for a pair of dyes linked to a calixarene scaffold. In systems where the geometry of the chormophore pair is not known a priori, the rate of energy transfer is estimated considering two limiting regimes, static and dynamic, that depict an oversimplified view of the mechanism. We make an extensive use of MD simulations in two different solvents to describe the effect of solvation and conformational motions on the rate of energy transfer. Moreover, we develop a fully dynamical model, based on Monte Carlo method, to analyze the characteristic timescales of such processes and compare them with the experimental picture. This work solved a major issue related to the characterization of RET rates in systems with high flexibility, emphasizing the importance of a dynamical approach for the description of complex decay mechanisms and opening up new opportunities for their theoretical treatment.



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virtual CpiC 2021 | Abstract

Structural and photoluminescence properties of carbon dots

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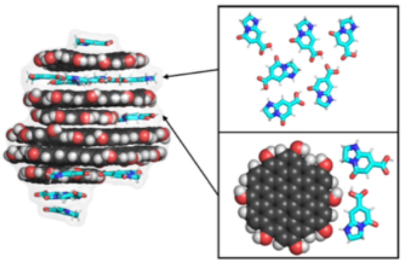
Carbon quantum dots (CQDs) belong to extensively studied nanomaterials with a very broad application potential resulting from their bright photoluminescence (PL), high (photo)stability, low toxicity and great biocompatibility. Their structure is quasi-spherical and can be made of graphene-like sheets stacked on each other with outer surface passivated by O- or N-containing functional groups.[1] This type of carbon dots (CDs) can be prepared from citric acid and diethylenediamine. During synthesis, various molecular fluorophores (MFs) were found in a final solution, such as 5-oxo-1,2,3,5-tetrahydroimidazo [1,2-α] pyridine-7-carboxylic acid, (IPCA).[1] Nevertheless, the design of CDs with tailored properties is still hampered by a fairly limited understanding of their PL, which stems from their rather complex structure and variability of the PL centers. Our theoretical calculations provided valuable insights into the structural organization of CQDs, and PL of MFs in gas and aqueous solution.[2,3,4] For the first time in the field, we performed molecular dynamics (MD) simulations of CQDs and we analyzed the stability and internal dynamics of various CQDs differing in size and surface functional groups.[2] Moreover, we characterized the stability and PL properties of IPCA complexes by combining QM and MD methods. Here we analyzed the UV absorption and fluorescence properties of the IPCA monomer and stacked IPCA dimers as basic models for the fluorescent centers in CDs.[3] Additionally, we employed MD simulations in order to investigate the nature of interactions of IPCA with CQDs in water and concluded that IPCAs showed a tendency to self-assemble and form seeds of CQDs during their synthesis. We also found out that IPCAs interacted with graphitic building blocks of CDs and incorporated into their structures via π-π stacking.[4] We believe that understanding the structure-optical properties relationship of CDs will help our understanding of PL properties of these nanosystems.



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Simulating liquid crystal self-assembly of oligonucleotides

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Liquid crystals (LCs) are well-known functional soft materials, whose structures can be found in several biological molecules. LC ordering of DNA was first observed in vitro for long double strands, but only quite recently it started being considered as a common arrangement for DNA oligomers. Several examples have been described in the literature, such as sequence-directed self-assembly[1], base stacking driven structures[2] and various form of LC long-range ordering[3]. In this context, computer simulations could complement experiments with detailed insight into the processes involved in self-organization. We attempted to reproduce the LC ordering obtained from a solution of single strand GCCG oligonucleotide at relatively high saline concentration (in the range 0.6 M to 2.0 M), until now only experimentally observed by Bellini and coworkers[4]. By means of Molecular Dynamic simulations and through the usage of OxDNA[5] as coarse-grained model of representation for DNA interactions, we successfully demonstrated the lyotropic behavior of the GCCG oligonucleotide. Self-assembly for short strands is a consequence of pairing and staking interactions: oligomers rapidly hybridize into duplexes, which in turn organize themselves in linear aggregates. As the saline concentration is enhanced, linear aggregates align and form LC phases. Specifically, we found that oligomers undergo three main phase order transitions: isotropic to nematic, nematic to columnar and eventually from columnar to a surprisingly more disordered phase. LC phases attribution and characterization were performed by combining the quantitative assessment of orientational and positional order along with the diffusion coefficient calculation, which reveled to be functional to the understanding of the high concentration isotropic phase.

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Quantum confinement effects in WO_3 nanoparticles: implication for photocatalysts design

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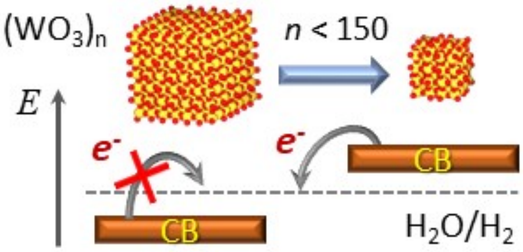
Tungsten trioxide (WO_3) derived nanostructures have emerged recently as new semiconductors for photocatalytic purposes due to their visible light absorption and high chemical stability, allowing to overcome some of the limitations presented by TiO_2 nanoparticles (NPs). Their widespread application, however, is still limited by the lack of fundamental knowledge about the main physical processes affecting their photoactivity. In this framework, we tackled the computational characterization of the electronic structure of realistic WO_3 NPs containing up to 1680 atoms, including different phases and morphologies, with the aim of drawing reliable structure-property relationships. Hence, we explored ground state properties of these NPs by means of Density Functional Theory (DFT) and *GW* calculations. More in detail, we used *GW* approximation for the smaller particles and derived reliable extrapolation procedures to approach the corresponding values for the larger NPs from less expensive DFT calculations. This strategy allowed us to elucidate which combinations of size and morphology are optimal to exploit this material in photocatalysis. From the point of view of morphology, cubic/nanosheet NPs were found to be energetically favoured at medium (n>50) and large (n>165) sizes respectively, whereas for smallest systems, rectangular/nanowires showed a larger stability. In all cases, the total energy reaches an asymptotic behaviour with respect to the particles size once these contain a few hundred units. Precisely, we found that in the regime previous to this asymptotic behaviour, quantum confinement effects modulate the electron injection driving forces with respect to H_2/H_2O reduction potential which opens a possible way to engineer their photoactivity.



Impact of Van der Waals interactions on structural and nonlinear optical properties of azobenzene switches

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Azobenzene derivatives are popular non linear optical photochromes because of their ability to convert between two conformational isomers, the stable trans and the metastable cis, with a large contrast in their first hyperpolarizability. Recently, the chemical functionalization of azobenzene molecules with bulky substituents has been shown to significantly impact their photochemical processes, due to intramolecular Van der Waals (VdW) interactions that stabilize the Z isomers [1]. In addition, VdW interactions are also expected to impact the non linear optical properties (NLOPs) of molecules with an azobenzene backbone.

In this work, we perform a theoretical study of the structure and NLOPs of a collection of azobenzene molecules symmetrically substituted in meta-position with functional groups of different bulkiness. We assess the performance of a large set of density functional approximations in reproducing the geometry, the relative energy and first hyperpolarizability of trans and cis isomers in comparison with ab initio calculations. Moreover, we analyze the individual contribution of the substituents on the response of this series of compounds, giving insights on the precise role of the functional groups responsible for dispersion interactions.

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O2

Stereochemistry & Direct Observation of Tautomerization of Single Hypericin Molecules

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Fluorescent organic bio-reporters are of great importance in bio- and biomedical applications, where targeted synthesis allows to design molecules which are able to probe specific nano-environments. The advance of spectroscopic and computational techniques in the past years now permits a unique, detailed nanoscopic insight into the interactions of the chromophore with its surrounding by combining single molecule spectroscopy with quantum chemistry calculations[1,2]. The computational results validate the experimental findings by imaging the absolute orientation of the single molecule transition dipole moments (TDMs) in the three-dimensional manner[2].

The current study is an important first step to develop a joint experimental-computational tool to probe nano-environmental effects at a single molecule level. With this insightful combination, an in-depth study of the well-defined molecules contributes to the elucidation of the structural complexity and specificity under different environmental conditions. The broad perspectives of bio- and biomedical applications seem to make the efforts worthwhile and we may be curious to witness their development over the coming years.

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On the structure–optical properties relationship in squaramide-based supramolecular polymers

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Self-assembly of molecules has become a powerful tool for the development of supramolecular nanoscale materials with a myriad of applications in photonics, electronics, and chemical biology among others.[1,2] In this context, the control over the self-assembly processes is essential for the development of well-defined nanostructures with the desired properties and functions. Herein, we present a theoretical study of the supramolecular polymerization of squaramide-based macrocycles. These macrocycles can be arranged in different supramolecular structures through a *Z*-*E* double bond isomerization. The distinct supramolecular polymers exhibit clear different optical properties which can be understood through a simple but extended Kasha model Hamiltonian.[3]

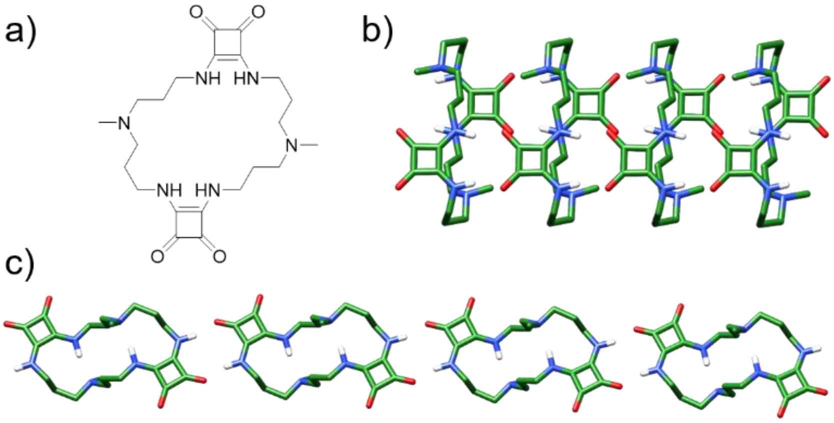

Figure 1. a) Chemical structure of the studied squaramide-based macrocycle. b) Structure of a head-to-tail aggregate c) Structure of a side-to-side aggregate

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C1

Excitonic Model for Strongly Coupled Multichromophoric Systems: The Electronic Circular Dichroism Spectra of Guanine Quadruplexes as Test Cases

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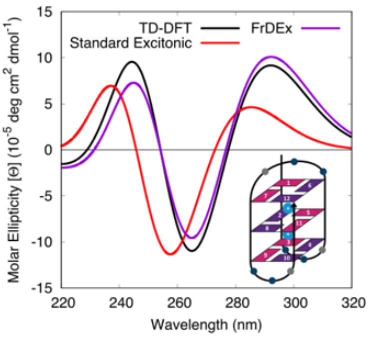
Excitonic Hamiltonians are widely employed cost-effective tools to model photoactivated processes in multichromophoric arrays. Here, we propose a general and flexible approach, based on fragment diabatization, which incorporates charge transfer states [1] and significantly increases the reliability of excitonic Hamiltonians for strongly coupled systems. This model (FrDEx) is used to compute the electronic circular dichroism and absorption spectra of two Guanine Quadruplex sequences (GQs), i.e., a fragment of the human telomeric sequence (Tel21, antiparallel), and (TGGGGT)$_4$ (TG4T, parallel). Calculations on different subsets of Tel21 and TG4T, from dimers to tetramers, show that FrDEx provides spectra close to the reference full quantum mechanical ones (obtained with time-dependent density functional theory), with significant improvements with respect to “standard” excitonic Hamiltonians [2]. Furthermore, these tests enable the most cost-effective procedure for the whole GQ to be determined. FrDEx spectra of Tel21 and TG4T are also in good agreement with the QM and experimental ones [3,4] and give access to interesting insights into the chemical−physical effects modulating the spectral signals. FrDEx could be profitably used to investigate many other biological and nanotechnological materials, from DNA to (opto)electronic polymers.



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Inverting the Singlet-Triplet Excitation Energy Gap in Triangle-Shaped Molecular Emitters

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The total harvesting of both singlet and triplet excitons is one of the main challenges to face in order to enhance the efficiency of organic light-emitting diodes. Design strategies such as TADF[1] (Thermally Activated Delayed Fluorescence) or the more recent Multi-Resonant[2] approach have represented prominent solutions to achieve this goal, by minimizing the energy gap between the singlet and triplet excited states to obtain a small, but still positive, ΔE_{ST} and promote a thermally activated up-conversion from T_1 to S_1. However, recent experimental and theoretical studies on triangle-shaped compounds, or triangulenes, suggested the potential inversion of the singlet and triplet energy order, violating the so-called Hund's rule, and providing a negative ΔE_{ST}[3][4].

This inversion originates from the interplay between the small singlet-triplet exchange interaction and electron correlation effects, arising from doubly excited configurations characterizing the excited states wavefunction.

In our work[5][6], we carried out a theoretical investigation on a set of triangulenes, doped with nitrogen and boron atoms, expected to have a negative ΔE_{ST}, assessing the effect of the dimension of the molecules and the doping pattern on their optical features. Unfortunately, the common TD-DFT methods, unable to deal with the double excitations, are not able to provide us with the right description for these compounds, and consequently, we need to rely on correlated wavefunction methods, such as CIS(D), SCS-CC2, SCS-ADC(2) and NEVPT2, which are key to predict the singlet-triplet inversion.

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C3

A Fragment Based Approach to the Quantum Dynamics of Multichromophoric Systems: Application to DNA Base Pairs

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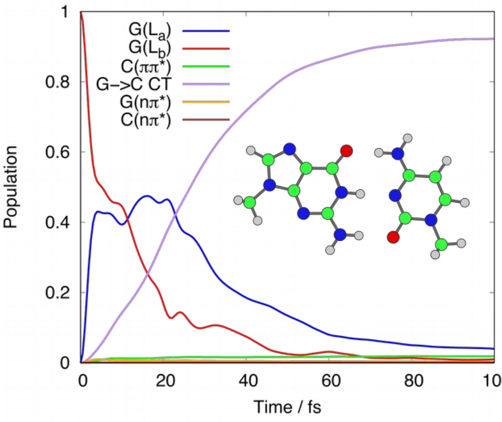
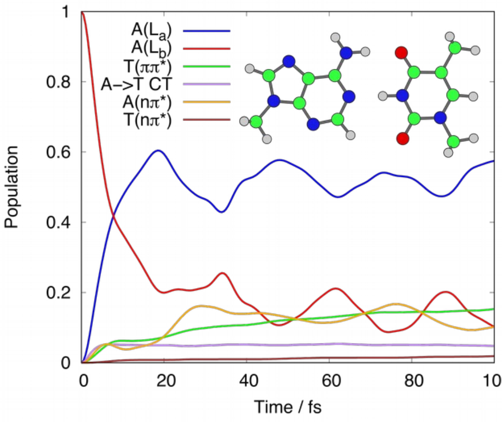
In this work we describe a fragment based diabatisation scheme, based on recent works,[1,2] that can parameterise a linear vibronic coupling (LVC) Hamiltonian for use with quantum dynamics calculations. The scheme takes as reference states local excitations (LEs) on individual fragments (such as bright ππ* or dark nπ* states) and one orbital transitions between fragments to describe charge transfer (CT) states. These reference states are then projected onto the multi-fragment species to obtain the energies and couplings necessary for the LVC model. This is described within the framework of TD-DFT, so that large systems may be tractably considered. As an initial test, the method is applied to the LE to CT dynamics of the guanine-cytosine and adenine-thymine Watson-Crick DNA base pairs, an archetypal example of multichromophoric species with individual LE structure. The dynamics are computed using the ML-MCTDH method, and the results from each base pair are compared and contrasted.





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Poster presentations

Understanding TADF: a joint experimental and theoretical study of DMAC-TRZ

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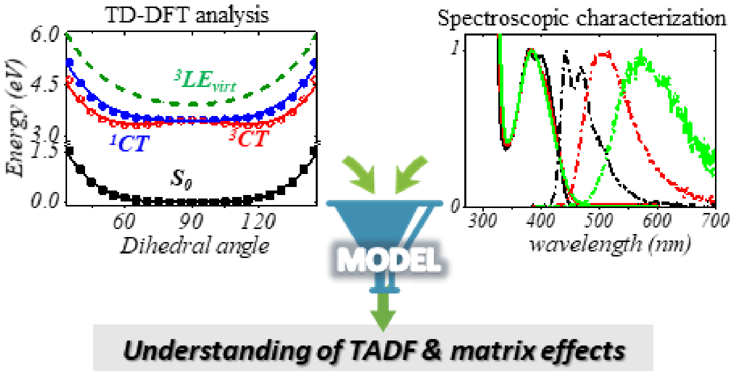
Thermally-activated delayed fluorescence (TADF) is a promising strategy to harvest triplets in OLED towards improved efficiency. Energy proximity between the lowest singlet (fluorescent) and triplet states (non-emissive) favors intersystem crossing and a subsequent reverse intersystem crossing (RISC) leading to delayed fluorescence and hence offering an effective way to harvest triplet states for OLED. The efficiency of TADF emitters is affected by several factors – (a) nature of excited states, (b) spin-orbit coupling, (c) conformational degree of freedom, (d) environmental effects, etc. A proper understanding of these interrelated factors is very much necessary to govern TADF as to improve the design of TADF materials. Towards this ambitious aim, we did an extensive spectroscopic study of a typical TADF dye (DMAC-TRZ) in liquid and glassy solvents. TD-DFT results for the same molecule in gas-phase and under an applied electric field are exploited to build a reliable model for the dye, rigorously validated against experiment. The model, accounting for charge transfer and local singlet and triplet states, spin–orbit coupling, conformational and vibrational degrees of freedom, sets the basis for a sound understanding of the photophysics of TADF dyes in different environments.[1] I will present how our model can be built to understand the nature of states and coupling between states. The concurrent role played by conformational degrees of freedom and the matrix polarizability in governing TADF will be also addressed.



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Electron transfer at bio-organic interfaces: A multiscale approach

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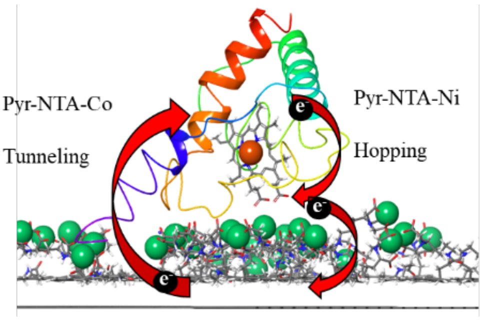
Construction of green nanodevices characterized by efficient direct electron transfer (DET) remains high priority in biotechnology and medicine. Tight electronic coupling of proteins to electrodes is essential for DET across the bio-organic interface. Rational modulation of this coupling depends on in-depth understanding of the intricate properties as well as the molecular mechanism of interfacial DET. Here, we report the dissecting the molecular mechanism of DET in a highly stable hybrid nanodevice in which a model electroactive protein, cytochrome c553 (cyt c553) was interfaced with single layer graphene via the conductive self-assembled monolayer (SAM) formed by pyrene-nitrilotriacetic acid (pyr-NTA) molecules chelated to transition metal redox centers. We demonstrate that efficient DET occurs between graphene and cyt c553 and whose kinetics and directionality depends on the metal incorporated into the bio-organic interface. Through combination of molecular dynamics and quantum mechanics/molecular mechanics (QM/MM) simulations we provide the mechanistic model of interfacial DET based on either tunneling or hopping of electrons between graphene, pyr-NTA-M2+ SAM and cyt c553 depending on the metal incorporated into the SAM. This fundamental discovery paves the way for the rational design of the optimal molecular interface between abiotic and biotic components of the high-performance green hybrid devices ranging from solar cells, optoelectronic nanosystems and solar-to-fuel electrochemical cells.



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Are large nanorings aromatic?

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Porphyrin nanorings are interesting compounds because they offer an end-free π-conjugated system with remarkable properties such as photophysical and guest-encapsulating.[1] Aromaticity is a multifold property[2] that is useful to understand the electronic structure of such belt-shaped π-systems. In fact, the larger the annulene, the less aromatic the molecule is expected to be and, for this reason, it is difficult to find large aromatic macrocycles.

Herein we perform a complete electronic structure study paying special attention to the (anti)aromaticity analysis and geometry assessment of a six-porphyrin nanoring template complex in four different oxidation states (neutral, tetracationic, hexacationic and dodecationic species).[3] In the latter work Anderson *et al* synthetized and analyzed the aromaticity of this nanoring structure arriving to the conclusion that haxacationic species was aromatic, tetracationic anitaromatic and the rest nonaromatic. However, in this work we demonstrate after the anaylsis of different aromaticity indices (*e.g.* NICS, ACID, HOMA, FLU or AV1245[4] $\mathrm{AV_{min}}$[4,5]) that the aromaticity of this large macrocyclic is questionable. We also provide evidence that the conclusions are highly sensible to the level of calculation comparing differents DFAs calculations.[6]

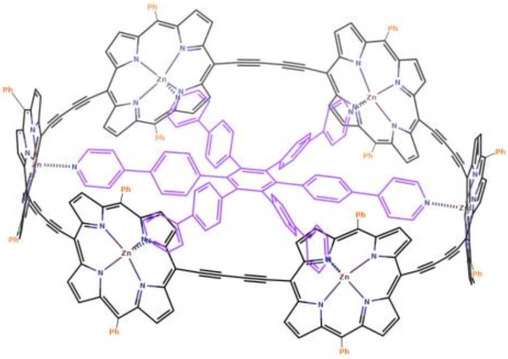

Image 1. Studied nanoring's structure.

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Vibronic Spectroscopy of π-Conjugated Systems with a Multitude of Coupled States. A Protocol Based on Quantum Dynamics Tested on Hexahelicene

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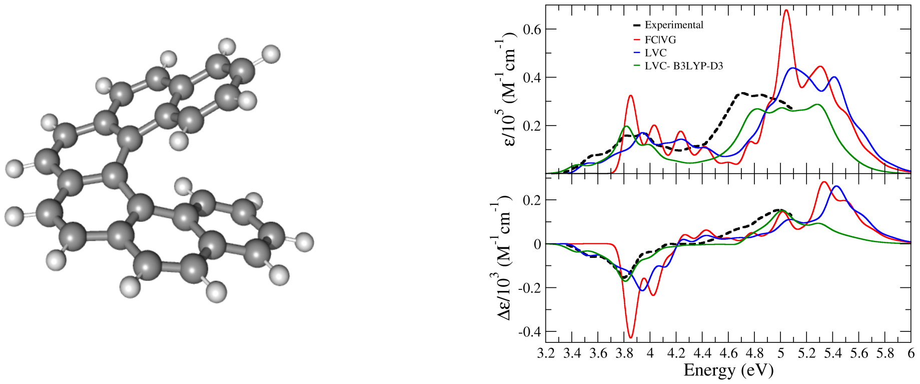
π-conjugated compounds are widely studied for the development of molecular electronics devices. To find potential candidates, their spectroscopic features are first modelled theoretically. However, these systems have a dense manifold of excited states, which are assumed independent for most of the popular quantum chemistry methods available. We show that the vibronic coupling among excited states are important to reproduce the absorption (ABS) and electronic circular dichroism (ECD) spectra of [6]helicene. This is done by performing quantum dynamics (QD) wavepacket propagations on diabatic potential energy surfaces described with a Linear Vibronic Coupling (LVC) model parametrized by a recently proposed diabatization procedure, based on maximum overlap.[1] QD simualtions are performed with Multi-Layer Multi-Configurational Time-Dependent Hartree (ML-MCTDH) method.[2] The results reproduce the full absorption and ECD spectra (3.0-5.0 eV, 415-250 nm) and show that one of the bands can only be explained by considering the nonadiabatic couplings, because it arises from the mixing of two electronic states. The limitations of standard "adiabatic" vibronic methods based on Frank-Condon and Frank-Condon Herzberg-Teller approaches are also highlighted. This protocol is very efficient and promising to make feasible the study of vibronic effects and the photophysics of even larger π-conjugated systems.



M-[6]helicene structure and ABS and ECD spectra calculated with the adiabatic FC|VG approach (M062X/6-31G(d)) and LVC parametrized with M062X/6-31G(d) and B3LYP-D3/6-31G(d) levels.

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Excited State Absorption of Conjugated Compounds: How Reliable is the “Single Excitation” Model?

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The understanding of the electronic excitation and deactivation processes are key factors for the application of conjugated compounds in optoelectronic devices. The detailed understanding of the properties of electronic excited states (ES) is a fundamental ingredient for the development of more efficient devices.

Pump-Probe Spectroscopy (PPS) is a powerful tool to analyze the photophysics in complex systems and has been successfully applied to study excited state absorption (ESA). Unfortunately, the analysis of PPS is difficult because of the multitude of optical probes and often need additional experiments. On the other hand, quantum-chemistry (QC) calculations of ESA are much less explored. Furthermore, didactic approaches to understand the constituting factors of the excitations are rather missing; methodology tests are scarce, and more advanced studies have not been carried out until now.

Since the excitation from ES can present strong configuration interaction (CI), it is expected that DFT based methods find difficulties in the description of the ordering of the states and in the excitation energies. In such cases, multiconfigurational (MCSCF) and multireference (MR) methods shows better results. The complete active space perturbation theory (CASPT2) method has been successfully applied for small conjugated systems, such as stilbene and thiophene. (1,2) Unfortunately, CASPT2 is size limited, since the computational cost makes impossible the application for medium to large size compounds.

Based on that, our group investigated the accuracy of a quadratic response (QR) TDDFT methodology applied to distyrylbenzene, a working horse conjugated compound of optical spectroscopy. The results showed a good agreement between the calculated ESA spectra and the PPS one. (3)

In this work, we present a comparison between QR-TDDFT and CASPT2 calculations for the excitations from the first ES (S_1). The results show that for the small system (bithiophene) QR-TDDFT fails since the main transition present a high contribution of double excitation (not computed by this method). Nevertheless, for terthiophene the QR-TDDFT can reproduce the main transition well.

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Conformational changes as driving force for phase recognition

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Laurdan and diphenylhexatriene (DPH) are ones of the most used fluorescent probes for lipid membrane phase recognition. By means of Molecular Dynamics and hybrid Quantum Mechanics – Molecular Mechanics (QM/MM) calculations, we compare the position, orientation and optical properties of these probe embedded in dipalmitoyl-phosphatidylcholine (DPPC) solid gel (So), dioleoylphosphatidylcholine (DOPC) liquid disordered (Ld) membranes, as well as in a liquid ordered (Lo) mixture of 2:1 Sphingomyelin and Cholesterol (SM/Chol) at room temperature.
Laurdan can take two conformations, depending on whether the carbonyl oxygen points toward the β-position of the naphthalene core (Conf-I) or to the α-position (Conf-II) [1]. We observe that Conf-I has an elongated form in DPPC (So), whereas Conf-II takes an L-shape. Moreover, our results show that in DPPC (So) no intermixing between the conformations is present, whereas it has been seen in a fluid environment such as DOPC (Ld) [2, 3]. Despite Laurdan's wide use as a solvatochromic probe, little is known regarding its use as molecular rotor. We prove now that information on the probe's conformation can be obtained through the optical properties, ranging from one-photon absorption over two-photon absorption to the first hyperpolarizability. Fluorescence decay and anisotropy analyses are performed as well and stress the importance of Laurdan's conformational versatility. As a molecular rotor, Laurdan can be used to probe biochemical processes that change the lipid orders in cell membranes.
With respect to DPH, the transition dipole moments and one-photon absorption spectra obtained in SM/Chol (Lo) differ largely from the ones calculated in DOPC (Ld) and DPPC (So) [4, 5]. The molecular conformation of DPH in SM/Chol is found to differ from the other environments. The two-photon absorption spectra and the ones obtained by hyper-Rayleigh scattering depend strongly on the environment. Finally, a stringent comparison of the fluorescence anisotropy decay and the fluorescence lifetime confirm the use of DPH to gain information upon the surrounding lipids and lipid phases. DPH might thus open the possibility to detect and analyze different biological environments based on its absorption and emission properties.

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Understanding Charge Transport Mechanisms of Ladder-type Heteroarenes: A joint Experimental and Theoretical Study

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In recent years, highly electron-efficient bithiophene imide-based ladder-type heteroarenes (BTI2-BTI5) have been synthesized[1,2], which present highly planar backbones with large π-conjugation lengths and reduced bangdgaps. However, despite their high planarity and encouraging electron mobility, these BTI-fused systems in OFETs, present a significant decrease of the charge transport properties upon increasing the building block length, which was an unexpected result. For a better interpretation of this behaviour, here we have investigated the influence of the molecular length and structure of these series of BTI-based semiconductors on the stabilization of charged states in solution and in the solid state. To this end, we used *in situ* UV/Vis/NIR spectroelectrochemistry and charge modulation spectroscopy (CMS), supported by density functional theory (DFT) calculations at different levels of theory[3]. DFT and TD-DFT calculations were conducted for both monomeric and π-dimeric species in solution by using PCM.

Interestingly, we found that charge stabilization in the shortest system of the series (BTI2) is strongly favored via a π-dimer formation (Figure 1) which, in addition to higher thin film microstructural ordering, results in a greater electron mobility in OFETs.

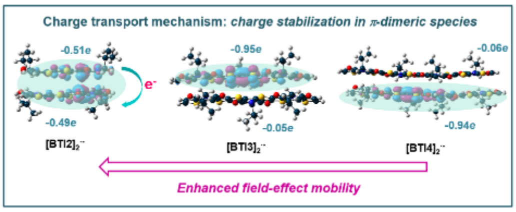

Figure 1. BTIn charge delocalization within the π-dimers.

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In silico Design of 2D Polymers based on C_3-symmetric Truxene-based Platforms

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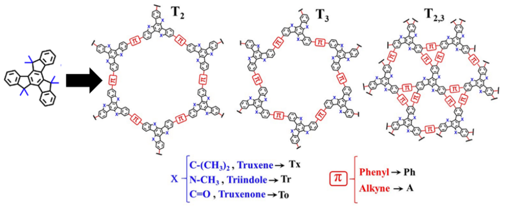
Expanding the π-conjugation has emerged as an efficient strategy to have large electron delocalization in 2D or 3D dimensions. In this sense, the design and sysnthesis of Covalent Organic Framework (COF) systems as semiconducting materials with enhanced transport dimensionality has been deeply investigated. These materials are constructed from the union of different covalently linked conjugated platforms and they have a wide range of analytical applications, such as adsorption and/or separation of certain compounds, catalysis or identification of analytes, among others.[1] On the other hand, the π-conjugated nature of these systems together with their extended 2D nature make them excellent candidates to be used in organic electronics or sensing applications.[2-3] Recently, in collaboration with the groups of Dr. Gómez-Lor and Dr. Martínez, we have theoretically investigate two-dimensional (2D) conjugated polymers based on C_3-symmetric truxene-based cores at the DFT level. In total, 27 different 2D polymers (Figure 1) have been exhaustively studied with the aim to explore the impact of the following effects on the electronic and charge-transport properties: (i) the nature of the conjugated platform, going from electron-rich truxene (Tx) and triindole (Tr) units to electron-deficient truxenone (To) cores, (ii) the spacing of the cores with different bridges, i.e., phenylene (Ph) or ethynylene (A) units, (iii) the linker position (2,7,12-substitution in the T_2 polymers and 3,8,13-substitution in T_3 polymers), and (iv) the increased number of π-bridges connecting the cores, from three linkers in T_2 and T_3 to six linkers in $T_{2,3}$.[4] Our results show that simultaneous manipulation of the pore surface size and band-gap engineering together with charge- transport parameters can be achieved in these truxene-based 2D polymers by fine-tuning their structural features, opening the doors for their subsequent synthesis and real application in organic electronic devices.



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Tau protein binding site in Alzheimer's disease for cationic luminescent ligands

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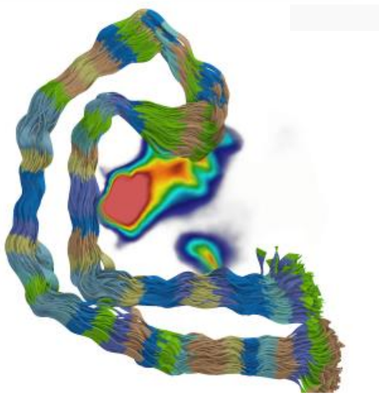
Intraneuronal Tau protein and extracellular Amyloid protein are considered major hallmarks for detecting Alzheimer's disease at an early stage.[1] The Tau protein, as compared to amyloid protein, has been studied sporadically due to a lack of atomistic details. In 2017, Fitzpatrick, et al. released the cryo em structure of Tau protein[2] , which helped carry out atomistic simulation and predict a probe's binding properties to Tau protein. It is crucial to know the binding sites within this protein for cationic and anionic probes to fine-tune a probe's binding. The current study proposes a strong binding site for the interaction between a cationic probe bTVBT4[3] and the Tau fibril based on unbiased MD simulation. In this site, the probe mainly interacts with amino acid residue ILE360, THR361, and HIS362 in four major binding modes. The results are corroborated by experimental studies.



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A reversible coarse grained model for truly accurate multi-scale simulations

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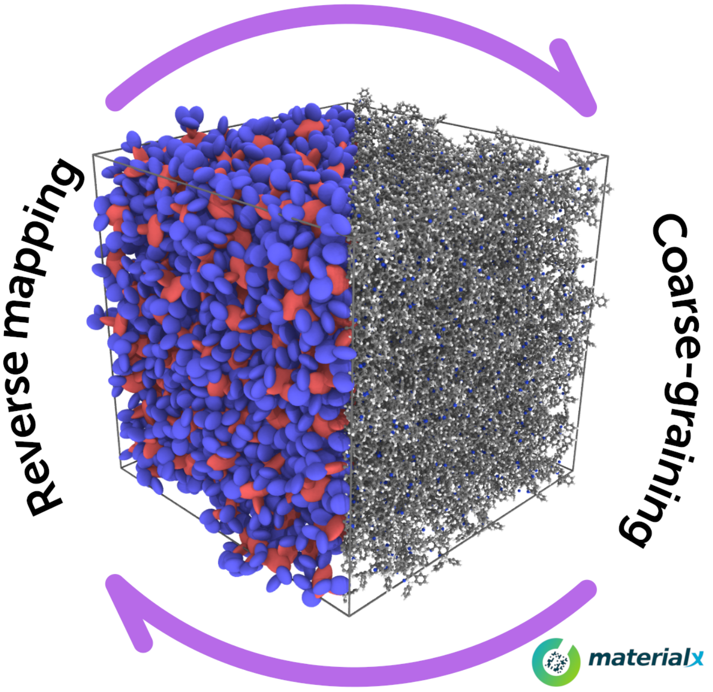
An innovative coarse grained (CG) model has been recently released for the description of complex organic molecules. This model is able to describe large-scale morphology (e.g. amorphous matrices, thin-films) with a structural accuracy comparable to that of more sophisticated approaches, yet at a fraction of the computational cost and time. Unlike most CG models, the presented one has the ability to reproduce the excluded volume of molecules at a level comparable to those of atomic force fields. This unique characteristic allows the reverse-mapping of atomic coordinates which are suitable to carry out electronic-structure calculations, capturing the complexity of real materials. The general characteristics, advantages and trade-offs of the model are presented, along with a selection of case studies in the field of organic electronics.



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Mechanisms and kinetics of free radical reactions with 5-bromouracil in neutral aqueous solutions

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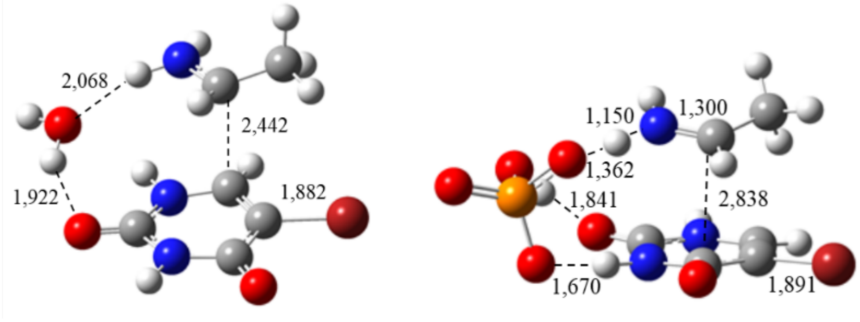
The reaction mechanisms and kinetics of free radical reactions with halogenated nucleobase 5-bromouracil, in non-buffered and buffered (bicarbonate and phosphate) aqueous solutions were investigated. This includes a study of the reactivity of C-centered α-aminoalkyl radicals: $^{\bullet}\mathrm{CH(CH_3)NH_2}$, $^{\bullet}\mathrm{CH(CH_3)NHCH_3}$, glycyl radical anion $^{\bullet}\mathrm{CH(NH_2)COO^-}$ and hydrogen atom ($\mathrm{H^{\bullet}}$) with 5-bromouracil. The radiosensitivity of halogenated nucleobases is of continuous interest because it is much enhanced relative to the parent nucleobases, which has potential clinical applications. Additionally, 5-bromouracil as a nucelobase analague is capable of inducing mautagenesis.[1]

For optimizing the stationary structures as well as to provide the energetics for the subsequent calculation of the reaction rate constants, the density functional theory (DFT/M06-2X) was employed. The solvent was initially described implicitly using the polarizable continuum model (PCM) and then the influence of explicit water molecules and buffers anions ($\mathrm{HCO_3^-}$, $\mathrm{HPO_4^{2-}}$) on the mechanisms and reaction energetics was explored. The reaction rate constants were calculated employing the conventional transition state theory and for the set of radical reactions, we investigated which types of exchange-correlation functionals produce the rate constants in best agreement with the measured ones.[1,2]

The dominant reaction mechanisms are mainly *ortho*- or *ipso*- additions to the double bond; denoted with respect to the Br atom, *o*-Ad and *i*-Ad. Although relatively unfeasible, the proton-coupled electron transfer mechanisms (PCET) can be observed in the presence of a basic buffers. PCET mechanisms receive a large attention since there is a large number of natural and electrochemical processes which crucially depend upon PCET.



TS-*o*-Ad **TS-PCET**

Figure 1. Transition state structures for reactions of $^{\bullet}\mathrm{CH(CH_3)NH_2}$ with 5-BrU in neutral aqueous solutions. PCM/M06-2X/6-311+G(2d,p); distances in Å.

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Analyzing SERS spectrum of 4-Cyanopyridine adsorbed on silver nanoparticles by means of DFT calculations

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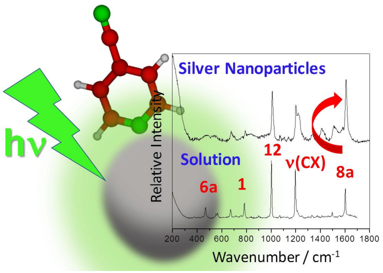
Surface Enhanced Raman Spectroscopy (SERS) has become a powerful technique to investigate the electronic structure of surface-molecule hybrid systems due to the huge enhancement of the Raman signal[1] exhibited by some aromatic molecules[2]. In this study the SERS spectrum of 4-cyanopyridine (4CNPy) was recorded on silver plasmonic nanoparticles and analysed by using Density Functional Theory (DFT) calculations performed at the B3LYP/LanL2DZ level of theory. Taking into account two interaction sites of the adsorbate, (aromatic Nitrogen, N, and nitrile group, CN), simple molecular models were proposed for metal-4CNPy surface complex with a silver cation (Ag+-4CNPy) or a neutral dimer (Ag2-4CNPy). The theoretical vibrational wavenumbers and intensities of both adsorbate and isolated species has been compared with the experimental SERS in presence and absence of chloride anions. The comparison between DFT predictions and experimental data indicates that 4CNPy adsorbs preferentially at neutral/charged active sites of silver nanoparticles through the nitrogen atom of the aromatic ring with a perpendicular orientation and that there are not dimers or reduction products.[3]



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Multimode dissipative quantum dynamics for polar dyes

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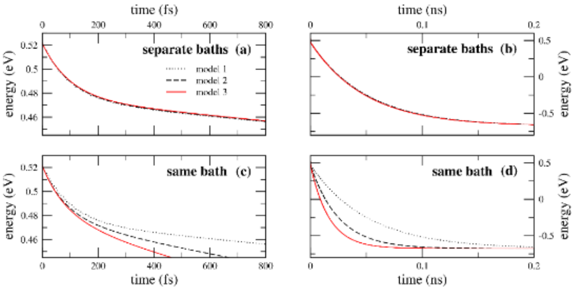
Modeling the relaxation of excited states is a crucial issue in spectroscopy since relaxation is the key to address dynamical processes in time-resolved spectroscopies as well as spectral bandshapes in steady-state spectra. Modeling energy dissipation in quantum systems is non-trivial, as one should account for the interaction of the system with its macroscopic environment, an impossible task in terms of model Hamiltonians, in view of the virtually infinite number of variables needed. The recent and challenging field of *open quantum-systems* faces this issue coupling the system, described by a quantum-mechanical Hamiltonian, to a bath that mimicks the environment in a simplified phenomenological approach. Validating the phenomenological models for open-quantum systems against experimental results is therefore of paramount importance to reliably describe the physics of quantum systems.

The relaxation of a single charge-tranfer D-π-A dye described by a two-level Hamiltonian and coupled to a single vibrational mode has successfully been modeled in ref[1] adopting the Redfield approach, where the bath is described as an infinite collection of quantum harmonic oscillators maintained at the thermal equilibrium linearly coupled to the vibrational coordinate of the dye.

In this work we test the validity of these results accounting for more than a single vibrational mode, addressing D-π-A systems with two and three molecular vibrations coupled to Redfield bath(s). The most delicate issue is the correct description of the coupling between the system and the bath. Indeed one may either couple all molecular vibrations to the same Redfield bath or couple each coordinate independently to a separate Redfield bath. We demonstrate that coupling all vibrational coordinates to the same Redfield bath imposes unphysical constraints on the dynamics of the different vibrational modes, so that the physically relevant model sees each coordinate independently coupled to a different Redfield bath. Results in ref[1] are robust against the number of vibrational degrees of freedom, confirming the power of this approach, able to account for the complex physics of relaxation following photoexcitation.



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Relationship between molecular, supramolecular, and optical properties of N-annulated perylene Bisimides aggregates

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Perylene bisimide (PBI) and its derivatives have aroused considerable attention due to their applications in diverse fields ranging from optical switches to organic light-emitting diodes (OLEDs).[1] PBIs are organic π-conjugated compounds and show excellent optical, photophysical, and optoelectronic properties. Furthermore, PBIs present different forms of aggregation due to peripheral substitutions, and the nature of these supramolecular aggregates plays a crucial role in the absorbance and fluorescence properties of the corresponding material.[2]

Here, we present a quantum-chemical characterization of the structural, electronic, and optical properties of PBI derivatives and their possible supramolecular aggregates by using the tight-binding semiempirical GFN2-xTB quantum-chemical method and its time-dependent variant (sTDA-xTB). The study has been performed on two PBI derivatives (Figure 1), which share the same π-conjugated core but different peripheral substituents attached to the imide positions (phenyl groups for **1** and ethyl benzoate groups for **2**). The change of the peripheral substituents has a strong effect on the aggregation and optical properties.

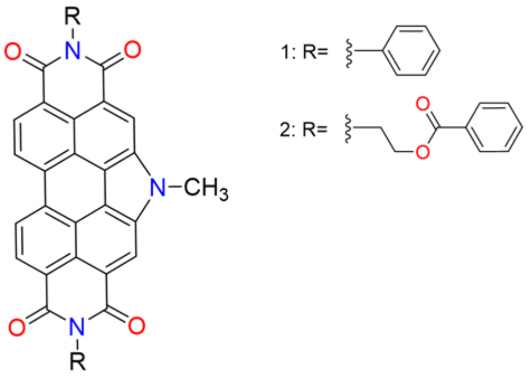

Figure 1. Chemical structure of the PBI derivatives.

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Unravelling calmodulin conformational ensemble from combined molecular dynamics and FRET simulations

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Förster resonance energy transfer (FRET) is a technique widely used as a spectroscopic ruler to measure distances in biosystems, and molecular simulations have emerged as an ideal complement to FRET due to its ability to explore the complex energy landscapes of biomolecules and provide structural models with atomic detail that can be compared with experiments.[1,2] These studies, however, typically rely on the approximations underlying Förster theory regarding donor-acceptor electronic coupling: a dipole-dipole term attenuated by a simple $1/n^2$ factor, where n is the refractive index of the medium, that accounts for screening effects exerted by the dielectric environment. In this work, we aim at developing a more rigorous theoretical framework to relate FRET experiments with conformational ensembles derived from classical molecular dynamics (MD) simulations. The approach is based on the polarizable quantum/molecular mechanics (QM/MM) model developed by our group, which uniquely allows to account for the impact of the heterogeneous polarizable environment on screening effects at an atomistic level. [3,4] We apply this strategy to study the Ca^{2+}-dependent conformational preferences of calmodulin (CaM), a ubiquitous protein that plays a major role in the transmission of calcium signals to target proteins in eukaryotes.[5] Our study allows to critically examine the accuracy of the MD ensembles simulated, to investigate the impact that different pairs of dyes on CaM conformational preferences, and to assess the impact of Förster limits in FRET derived distances of proteins.

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Intramolecular Singlet Fission in Homo-conjugated Dimers

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Singlet fission (SF) is a photophysical process where a spin singlet excited state splits into two spin-triplet states through an intermediate multiexcitonic state that corresponds to a correlated triplet-pair state.[1,3]

$$S_1 \rightleftharpoons {}^1TT \rightleftharpoons T_1 + T_1$$

Homo-conjugated systems are organic molecules in which two or more π-moieties are separated by a non-conjugating group.[2] Homo-conjugation results in a unique arrangement of conjugated fragments providing a novel way to chemically connect chromophoric units and control their electronic interaction. These properties might be of great use in singlet fission (SF), since optimal electronic coupling is a key ingredient for the efficient generation of two independent triplets from a singlet exciton.[1]

In this work, we employ different computational chemistry tools within the framework of Density Functional Theory and Wave Function Theory to identify the nature of the low-lying electronic states, characterize the particularities of electronic coupling in homo-conjugated systems, describe the intrachromophoric coupling and predict the overall viability of intramolecular SF in these type of covalent dimers.

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Quinoidal Structures on Resonant Transport in Single-Molecule Junctions

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Molecules provide almost unlimited design possibilities to modulate the charge transport at the quantum level. Among them, the alternation of electron-rich (D), and strong electron-deficient quinoid (A) units in π-conjugated molecules, constitutes a riveting approach for achieving outstanding conductance values in functional single-molecule devices through a resonant transport mechanism (within reasonable biases).
While in the D-A scheme, the quinoidal character induced by intramolecular charge D→A transfer (ICT), promotes the frontier molecular orbitals approach to the electrode Fermi level, and thus, a reduction of the charge injection barrier. The incorporation of a quinoidal structure as an electron-withdrawing unit can lower the injection barrier even further, achieving high conductance through a resonant transport mechanism. [1]
In this contribution, we highlight the relevance of quinoid structures, and especially the quinoidal resonance forms stabilized by aromatic-substructures, on the transport properties in *gold-molecule-gold* junctions. In this regard, we consider a series of D-A-D molecules based on thienoquinoid with carbonil termini electron-withdrawing groups as strong quinoid A units, and thiophene motifs acting as D groups, flanked by (-SMe) end groups to allow the anchoring to gold electrodes. These quinoid units have been previously investigated and proposed as strong A groups for the creation of very small bandgap polymers,[2] but have been unexplored into single-molecule electronic devices.
Non-Equilibrium Green´s Function (NEGF) formalism coupled to DFT is used to determine the energy-dependent transmission functions, T(E), as well as, the electronic current (I) and conductance (G) through the Landauer-Büttiker formalism.

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Evaluating the Role of Intermolecular Interactions in Piezochromic Materials by Raman Spectroscopy and DFT Calculations

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Piezochromic materials, which show colour changes resulting from external pressure or mechanical grinding, are of great interest from a scientific viewpoint owing to their potential applications as pressure-sensing and optical-recording systems.[1] It has been discovered solid-state fluorescence properties and piezochromic luminescence in a family of 9,10-Bis((E)-n-(pyrid-2-yl)vinyl)anthracene, BPnVA (n=2 orto-,3 metha- and 4 para-) compounds, see Figure 1.[2] The crystal structures indicate that the three compounds with varying position of the nitrogen on the external pyridyl exhibit different molecular packing modes. In this work, we aim at providing further insight into the interplay performed by the molecular and supramolecular structural changes and the luminescence changes observed under pressure and variable temperature. To this end, we will use a combined experimental-theoretical approach that links pressure and temperature dependant raman spectroscopy with DFT calculations of the single molecule and the crystalline structure.

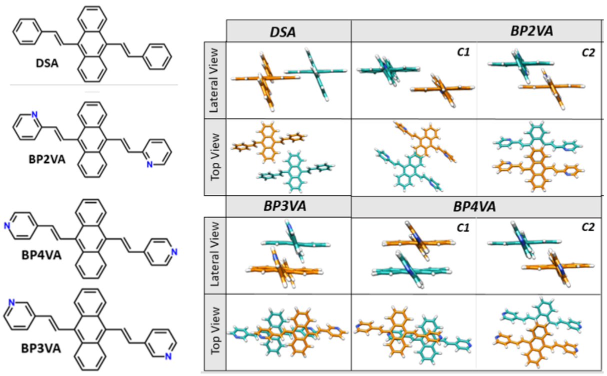

Figure 1. Chemical structures (a) and crystal packing (b) of the molecules under study.

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Thermally-activated delayed fluorescence: a critical assessment of environmental effects on the singlet-triplet energy gap

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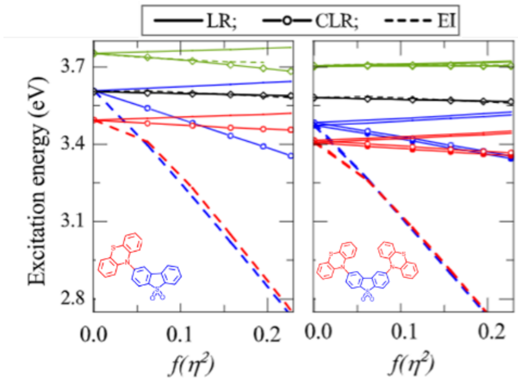
Thermally-activated delayed fluorescence (TADF) is one of the most promising triplet harvesting strategies to increase the efficiency of organic light emitting devices. The effective design of TADF dyes requires the precise control of two tiny energies: the singlet-triplet gap, that has to be maintained within thermal energy, and the strength of spin-orbit coupling. A subtle interplay among low-energy excited states having dominant charge-transfer and local character then governs TADF efficiency, making models for environmental effects both crucial and challenging. The use of implicit solvation models such as the polarizable continuum model (PCM) is widespread due to their efficiency and availability in most quantum chemistry packages. However, when it comes to fast (electronic) solvent response following electronic transitions in the solute, current PCM implementations implicitly rely on an adiabatic approximation.

In this work the consequences of such an approximation are critically evaluated focusing on relative energies of low-lying excited singlet and triplet states in TADF dyes and accounting for three PCM approximation schemes for fast solvation: the linear response (LR), the corrected linear response (CLR) and external iteration (EI). Relevant properties wildly depend on the adopted approximation scheme and unphysical results are in some cases obtained. Finally, a few state model approach is adopted to show how unphysical results are cured in the antiadiabatic approach to fast solvation proposed in Ref. 1.



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