

# 2020

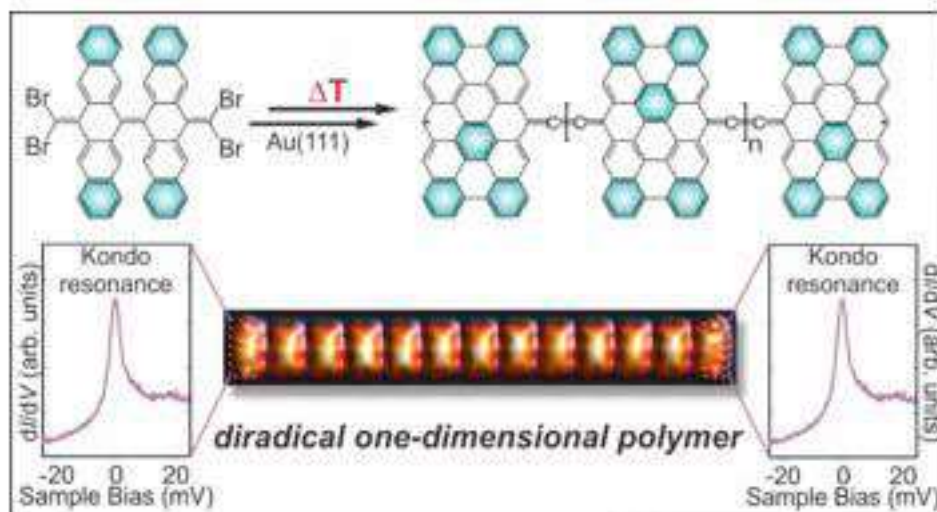


## ANNUAL REPORT 2020

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## RESEARCH PAPERS

1) A. Sánchez-Grande, J. I. Urgel, A. Cahlik, J. Santos, S. Edalatmanesh, E. Rodríguez-Sánchez, K. Lauwaet, P. Mutombo, D. Nachtigallová, R. Nieman, H. Lischka, B. de la Torre, R. Miranda, O. Gröning, N. Martín, P. Jelínek, D. Écija, "Diradical organic one-dimensional polymers synthesized on a metallic surface", *Angew. Chem. Int. Ed.*, **2020**, *59*, 17594-17599 - [doi.org/10.1002/anie.202006276](https://doi.org/10.1002/anie.202006276)



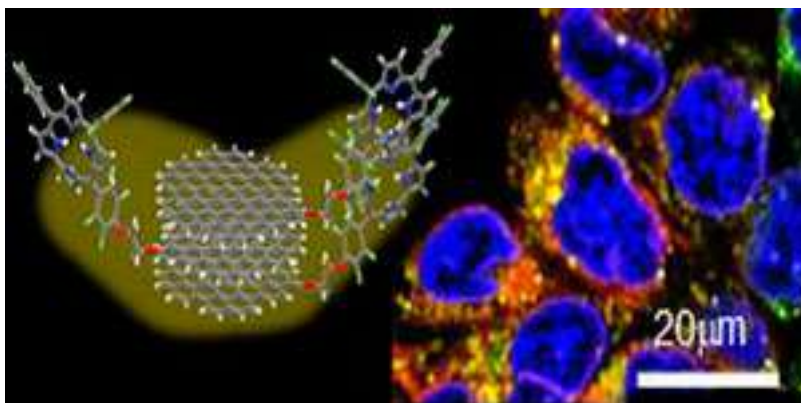
We report on the synthesis and characterization of atomically precise one-dimensional diradical peripentacene polymers on a Au(111) surface. By means of high-resolution scanning probe microscopy complemented by theoretical simulations, we provide evidence of their magnetic properties, which arise from the presence of two unpaired spins at their termini. Additionally, we probe a transition of their magnetic properties related to the length of the polymer. Peripentacene dimers exhibit an antiferromagnetic ( $S=0$ ) singlet ground state. They are characterized by singlet–triplet spin-flip inelastic excitations with an effective exchange coupling ( $J_{\text{eff}}$ ) of 2.5 meV, whereas trimers and longer peripentacene polymers reveal a paramagnetic nature and feature Kondo fingerprints at each terminus due to the unpaired spin. Our work provides access to the precise fabrication of polymers featuring diradical character which are potentially useful in carbon-based optoelectronics and spintronics.

2) "Ciamician-Gonzalez Lectureship" to Prof. Nazario Martín. *Angew. Chem. Int. Ed.* **2020**, *59*, 533



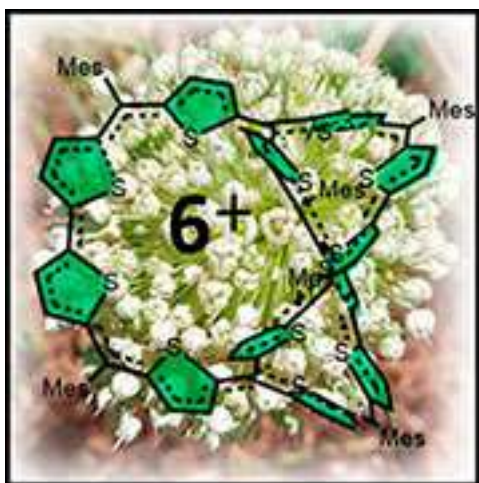
La Sociedad de Química de Italia reconoce a través de este galardón su trabajo en el campo de la química orgánica de nuevos materiales. El Catedrático en la Universidad Complutense de Madrid y subdirector del IMDEANanociencias, Nazario Martín, suma un reconocimiento más a su prolífica carrera en la investigación química. En esta ocasión, la Sociedad Química italiana le ha concedido el galardón Ciamician-González Lectureship 2019. El jurado presidido por el Prof. Salvatore Coluccia del Comité de Relaciones Internacionales SCI y formado por los profesores Gaetano Guerra, Gianluca Maria Farinola y Alberto Credi han acordado otorgarle el galardón "en reconocimiento por su extraordinaria contribución en el campo de la química orgánica de nuevos materiales. Sus resultados continúan siendo fuente de inspiración de nuevas generaciones de investigadores". El profesor Nazario Martín será invitado a exponer su trabajo en tres universidades o institutos de investigación en Italia durante este año 2019.

3) C. I. M. Santos, L. Rodríguez-Pérez, G. Gonçalves, S. N. Pinto, M. Melle-Franco, P. A. A. P. Marques, M. A. F. Faustino, M. A. Herranz, N. Martin, M. G. P. M. S. Neves, J. M. G. Martinho, E. M. S. Maçôas, "Novel hybrids based on graphene quantum dots covalently linked to glycol corroles for multiphoton bioimaging", *Carbon*, **2020**, *166*, 164-174 – doi: [org/10.1016/j.carbon.2020.04.012](https://doi.org/10.1016/j.carbon.2020.04.012)



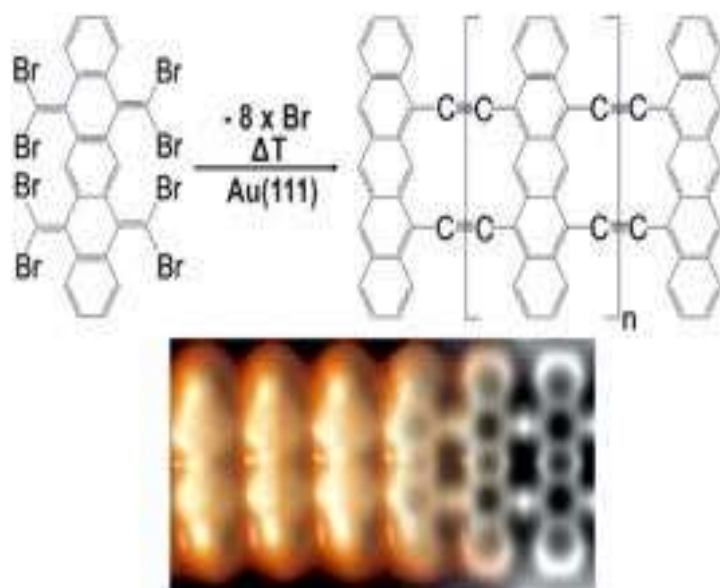
Graphene quantum dots (GQDs) possess excellent optical properties, high photostability, aqueous solubility and bio-compatibility. The presence of carboxyl and hydroxyl groups on GQDs surface and edges provides an excellent opportunity to explore them as anchoring units for covalent functionalization. In addition, the nonlinear optical response of GQDs allows the development of optical sensors operating in biological media. To evaluate the possibility of using GQDs to introduce a hydrophobic sensing unit inside animal cells and to add a nonlinear response to the sensing unit we prepared a novel hybrid based on GQDs covalently linked to corrole units bearing a glycol branch. Covalent functionalization was supported by X-ray photoelectron spectroscopy (XPS), Raman and Fourier transform infrared (FTIR) spectroscopy. Both the height and the diameter of the hybrid showed distributions peaking below 4 nm. The UV-vis absorption and emission spectra of the hybrids were additive with respect to that of the GQDs and the corrole. Insights about the most stable conformation of the corrole with respect to the GQDs core was provided by in silico studies using a model structure. The internalization and distribution of the hybrids in live animal cells was evaluated in human breast adenocarcinoma cell line (MCF-7 cells) using confocal and multiphoton microscopy. Notably, multiphoton microscopy allowed for image collection using nonlinear excitation in the near-infrared and emission in the red part of the visible spectra.

4) J. Casado and N. Martín, "The New "Noble Gas" Molecule: A Molecular Trip beyond Atoms", *Chem* **2020**, *6*, 1514-1516 - DOI: [10.1016/j.chempr.2020.06.009](https://doi.org/10.1016/j.chempr.2020.06.009)



The synthesis and characterization of three novel HTMs with different highest occupied molecular orbital (HOMO) energy levels and their performances in MAPbI<sub>3</sub>-based devices in comparison with Spiro-OMeTAD is reported. Without systematic optimization, the HTMs performed well. The devices delivered fill factors comparable to the one with Spiro-OMeTAD but suffered from short-circuit current (JSC). Interestingly, despite the significant differences in HOMO energy levels, all three HTMs generated the same open-circuit voltage (VOC). We explored the performance limiting factors of the HTMs by simple transient photovoltage/photocurrent (TPV/TPC) measurements along with drift-diffusion simulations. We found no correlation between HOMO energy levels of the HTMs and VOC of the devices. Performances of the devices are limited by high trap density as well as low carrier mobility of the HTMs, and by the shunts present in the devices. Furthermore, the high trap density and low carrier mobility of the HTM are found to induce ion migration effect in the device causing slow decaying components in TPV/TPC. Nevertheless, it is confirmed that JSC and VOC, measured at steady state, are not influenced by the ion migration effect. These HTMs can be improved further by optimizing their conductivity, trap density, morphology, and can be used as alternatives to Spiro-OMeTAD or other expensive, synthetically challenging HTMs. The simple and inexpensive approach presented in this work can also be applied for effectively evaluating charge transporting materials for perovskite solar cells.

5) K. Biswas, J. I. Urgel, A. Sánchez-Grande, S. Edalatmanesh, J. Santos, B. Cirera, P. Mutombo, K. Lauwaet, R. Miranda, P. Jelínek, N. Martín, D. Écija, "On-surface synthesis of doubly-linked one-dimensional pentacene ladder polymers", *Chem. Commun.*, **2020** - DOI: [10.1039/D0CC06865A](https://doi.org/10.1039/D0CC06865A)



On-surface synthesis has recently become an essential approach toward the formation of carbon-based nanostructures. Special emphasis is set on the synthesis of  $\pi$ -conjugated polymers taking into consideration their relevance and potential in organic electronics, optoelectronics and spintronics. Here, we report the on-surface synthesis of conjugated ladder polymers consisting of pentacene units doubly-linked via ethynylene-like bonds on the Au(111) surface under ultra-high vacuum conditions. To this aim, we have sublimed pentacene-like precursors equipped with four  $:\text{CBr}_2$  functional groups to steer the desired reaction upon annealing on the surface. The atomically precise structure of the obtained polymers has been unambiguously characterized via low-temperature scanning tunneling microscopy and non-contact atomic force microscopy. In addition, scanning tunneling spectroscopy complemented with density-functional theory calculations reveal the narrow bandgap of the polymer. Our results provide potential for the synthesis of  $\pi$ -conjugated polymers with prospects in functional carbon-based nanomaterials that exploit multiple connections between molecular backbones.

6) N. Martín, N. Tagmatarchis, Q. H. Wang, X. Zhang, Eds. "Chemical Functionalization of 2D Materials", *Chem. Eur. J.* **2020**, *26*, 6292 – 6295 – DOI: [doi.org/10.1002/chem.202001304](https://doi.org/10.1002/chem.202001304)



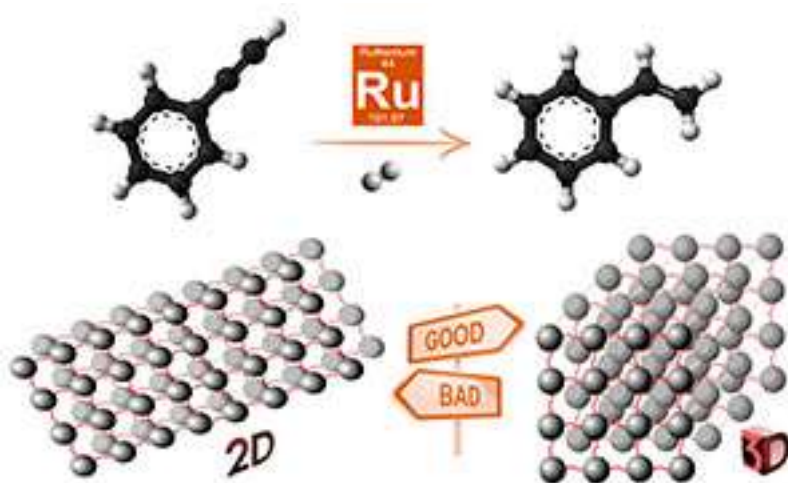
**Figure 1.** From left to right: Nazario Martin, Nikos Tagmatarchis, Qing Hua Wang, Xiaoyan Zhang.

This Special Issue of Chemistry–A European Journal is dedicated to the Chemical Functionalization of 2D Materials, and features some great contributions from experts in the field of 2D materials. This issue was originally assembled to support the Symposium G "Chemical Functionalization of 2D Materials" at the European Materials Research Society (E-



MRS) 2020 Spring Meeting, which was originally scheduled to be held in Strasbourg, France, from May 25th to 29th, 2020. Although the E-MRS 2020 Spring Meeting has been cancelled due to the COVID-19 outbreak, the publication of this Special Issue has proceeded and has become even more important as the contributors discuss diverse and timely research themes related to 2D materials. In this Editorial, a brief overview of the different types of 2D materials is given, together with the chemical functionalization schemes that can be applied to them to achieve new properties as well as enable improved performance in applications. Some of the articles featured in this Special Issue are also highlighted, with the hope that they will inspire readers and further advance the field.

7) Y. Min, F. Leng, B. F. Machado, P. Lecante, P. Roblin, H. Martinez, T. Theussl, A. Casu, A. Falqui, M. Barcenilla, S. Coco, B. M. Illescas, N. Martin, M. R. Axet, P. Serp. "2D and 3D Ruthenium Nanoparticle Covalent Assemblies for Phenyl Acetylene Hydrogenation", *Eur. J. Inorg. Chem.* **2020**, 5926-5937 - [doi.org/10.1002/ejic.202000698](https://doi.org/10.1002/ejic.202000698).



The bottom-up covalent assembly of metallic nanoparticles (NP) represents one of the innovative tools in nanotechnology to build functional heterostructures, with the resulting assemblies showing superior collective properties over the individual NP for a broad range of applications. The ability to control the dimensionality of the assembly is one of the major challenges in designing and understanding these advanced materials. Here, two new organic linkers were used as building blocks in order to guide the organization of Ru NP into two- or three-dimensional covalent assemblies. The use of a hexa-adduct functionalized C60 leads to the formation of 3D networks of 2.2 nm Ru NP presenting an interparticle distance of 3.0 nm, and the use of a planar carboxylic acid triphenylene derivative allows the synthesis of 2D networks of 1.9 nm Ru NP with an interparticle distance of 3.1 nm. The Ru NP networks were found to be active catalysts for the selective hydrogenation of phenylacetylene, reaching good selectivity toward styrene. Overall, we demonstrated that catalyst performances are significantly affected by the dimensionality (2D vs. 3D) of the heterostructures, which can be rationalized based on confinement effects.

8) L. Almagro, R. Lemus, K. Makowski, H. Rodríguez, O. Ortiz, W. Cáceres, M. A. Herranz, D. Molero, R. Martínez-Álvarez, M. Suárez, N. Martín, "[60]Fullerene Hybrids Bearing Steroid Wings: A Joint Experimental and Theoretical Investigation", *Eur. J. Org. Chem.* **2020**, 5926-5937 [doi: 10.1002/ejoc.202000989](https://doi.org/10.1002/ejoc.202000989).

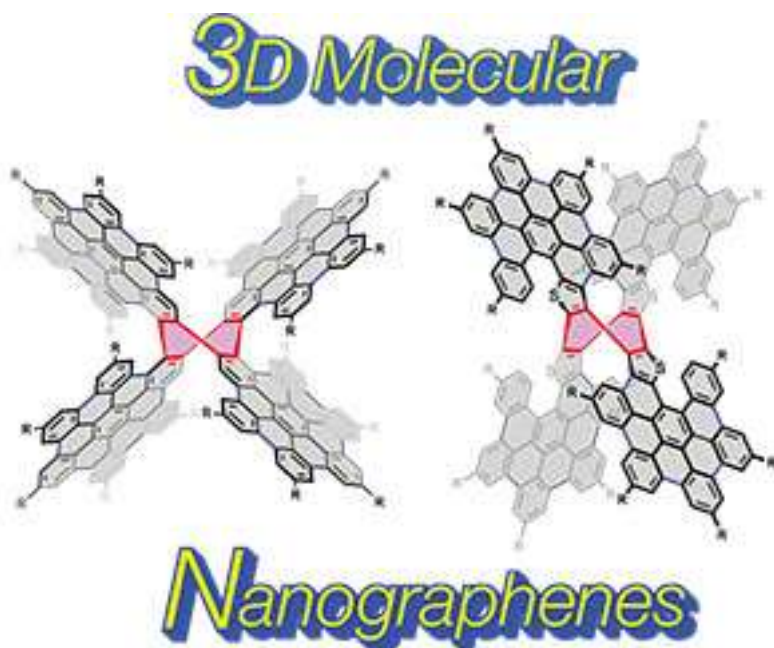


Novel [60]fullerene-steroid hybrids have been synthesized by Bingel–Hirsch cyclopropanation reaction between C<sub>60</sub> and steroid malonates, leading to conjugates in which a [60]fullerene unit is connected to one or two dehydroepiandrosterone moieties, an important naturally occurring steroid hormone. The obtained derivatives have been fully characterized by a whole set of instrumental techniques in order to determine their chemical structure. Moreover, their electrochemical properties, investigated by cyclic voltammetry, revealed the presence of three reversible reduction waves for both hybrids. Furthermore, Transmission Electron Microscopy studies allowed to determine the morphology and size of the fullerene hybrids in aqueous solution, showing a tendency to organize into spherical nanoscale structures. Theoretical calculations using the DFT-PBE method and 6-311G(d,p) basis set, were performed to predict the most stable conformations for the synthesized compounds, and to determine the factors that control the geometry of these hybrid molecules. In addition, parameters such as polarity, and lipophilicity were estimated. The obtained results corroborate the predicted activity against HIV-1 protease as suggested by molecular docking simulation.

9) N. Martín, "Jean-Pierre Sauvage: The Lord of the Rings (II)", *Eur. J. Org. Chem.*, **2020**, 2007-2011 - doi: [doi.org/10.1002/ejoc.202000404](https://doi.org/10.1002/ejoc.202000404)



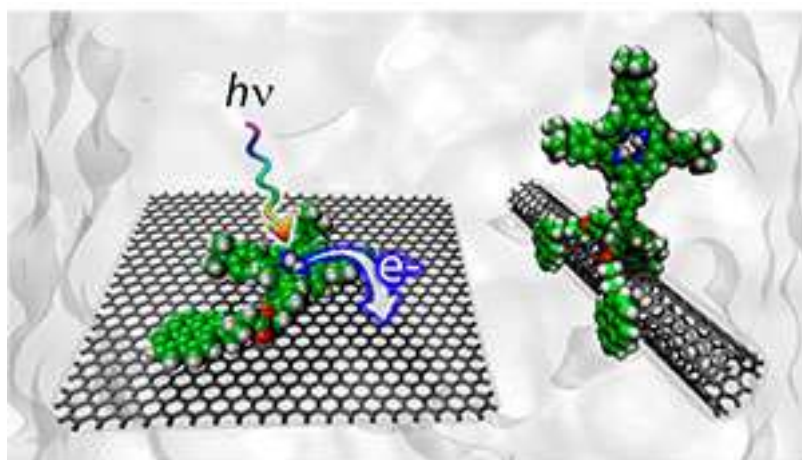
10) J. Urieta-Mora, M. Krug, W. Alex, J. Perles, I. Fernández, A. Molina-Ontoria, D. M. Guldi, N. Martín, "Homo and Hetero Molecular 3D Nanographenes Employing a Cyclooctatetraene Scaffold", *J. Am. Chem. Soc.*, **2020**, *142*, 4162–4172 - [doi: 10.1021/jacs.9b10203](https://doi.org/10.1021/jacs.9b10203)



Two novel homo and hetero three-dimensional nanographenes, NG1 and NG2, featuring a cyclooctatetraene core are designed, synthesized, and characterized. A concise and efficient bottom-up methodology was employed during which 24 new carbon–carbon bonds were formed. By means of a Scholl reaction nanographenes with 53 fused rings are realized, which exhibited good solubility in common organic solvents. The resulting saddle-like structures of NG1 and NG2 are electron-rich and show good chemical and electrochemical stability. Their molecular structures are fully elucidated by single-crystal X-ray crystallography. From their crystal structure analysis is concluded that both nanographenes are chiral and crystallize as a racemic mixture. Our work was rounded-off by excited state investigations such as electron and energy transfer with electron-acceptors and -donors.

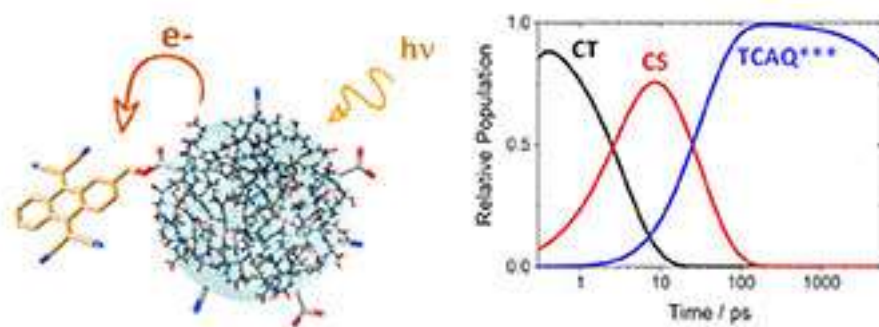


11) M. Garrido, M. K. Volland, P. W. Münich, L. Rodríguez-Pérez, J. Calbo, E. Ortí, M. A. Herranz, N. Martín, D. M. Guldi, "Mono- and Tripodal Porphyrins: Investigation on the Influence of the Number of Pyrene Anchors in Carbon Nanotube and Graphene Hybrids", *J. Am. Chem. Soc.* **2020**, *142*, 1895-1903 - doi: [10.1021/jac.9b10772](https://doi.org/10.1021/jac.9b10772)



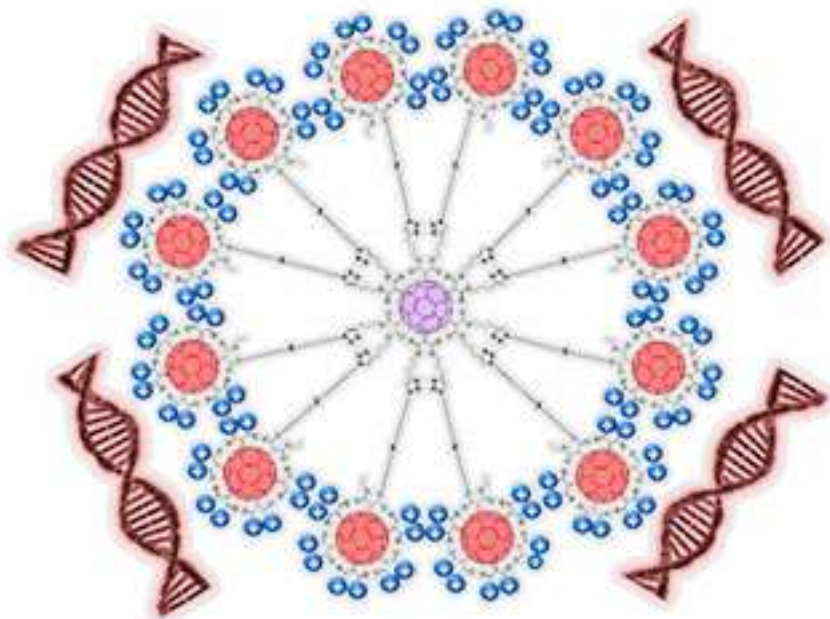
A series of molecular precursors, containing one (1 and 3) or three (2 and 4) pyrene anchors, covalently linked to porphyrins (free base or Zn), were prepared and characterized. All of them enable their  $\pi$ - $\pi$  stacking onto low-dimensional nanocarbons including single-walled carbon nanotubes (SWCNTs) and nanographene (NG), their individualization, and their characterization. Microscopic (TEM, AFM) and spectroscopic (steady-state UV-vis and fluorescence, spectroelectrochemistry, and transient absorption measurements) techniques were at the forefront of the characterizations and were complemented by Raman spectroscopy and theoretical calculations. Of great importance is the Raman analysis, which corroborated n-doping of the nanocarbons due to the interactions with 1-4 when probed in the solid state. In solution, the situation is, however, quite different. Efficient charge separation was only observed for the graphene-based system NG/3.

12) A. Ferrer-Ruiz, T. Scharl, L. Rodríguez-Pérez, A. Cadranet, M. A. Herranz, N. Martín, D. M. Guldi, "Assessing the Photoinduced Electron-Donating Behavior of Carbon Nanodots in Nanoconjugates", *J. Am. Chem. Soc.* **2020**, *142*, 20324-20328- doi:[10.1021/jacs.0c10132](https://doi.org/10.1021/jacs.0c10132)



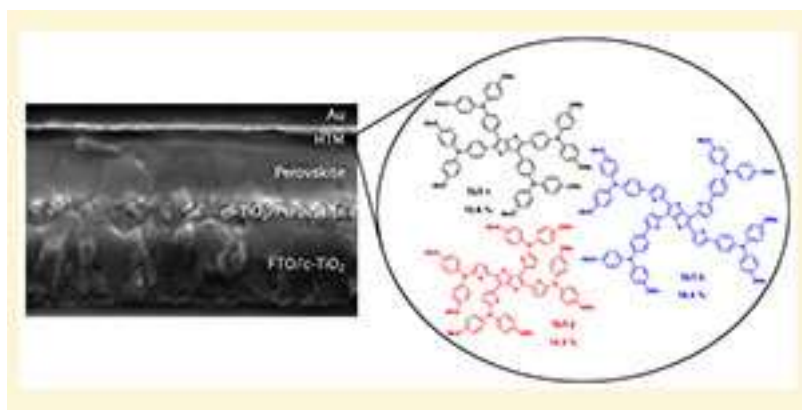
Carbon nanodots (CNDs) undergo electron transfer in different scenarios. Previous studies have mainly focused on the electron-accepting features of CNDs in covalently linked donor-acceptor nanoconjugates. In view of this, we decided to carry out in this study the formation of covalently linked nanoconjugates that feature electron-donating pressure synthesized carbon nanodots (pCNDs) and electron-accepting 11,11,12,12-tetracyano-9,10-anthra-p-quinodimethane (TCAQ): pCND-TCAQ. The stability of the one-electron reduced form of TCAQ renders it the acceptor of choice. Detailed structural and electrochemical investigations allowed





Non-viral nucleic acid vectors able to display high transfection efficiencies with low toxicity and overcoming the multiple biological barriers are needed to further develop the clinical applications of gene therapy. The synthesis of hexakis-adducts of [60]fullerene endowed with 12, 24 and 36 positive ammonium groups and a tridecafullerene appended with 120 positive charges has been performed. The delivery of a plasmid containing the green fluorescent protein (EGFP) gene into HEK293 (Human Embryonic Kidney) cells resulting in effective gene expression has demonstrated the efficacy of these compounds to form polyplexes with DNA. Particularly, giant tridecafullerene macromolecules have shown higher efficiency in the complexation and transfection of DNA. Thus, they can be considered as promising non-viral vectors for transfection purposes.

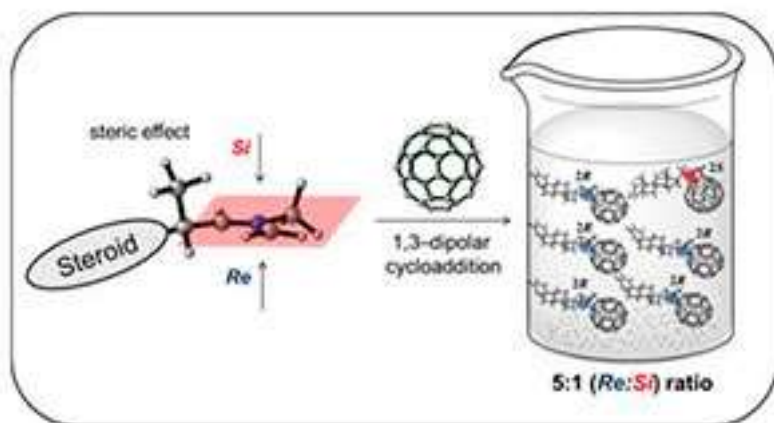
15) J. Urieta-Mora, I. García-Benito, I. Zimmermann, J. Aragón, A. Molina-Ontoria, E. Ortí, N. Martín, M. K. Nazeeruddin, "Tetrasubstituted Thieno[3,2-b]thiophenes as Hole-Transporting Materials for Perovskite Solar Cells", *J. Org. Chem.* **2020**, *85*, 224-233 - doi: [10.1021/acs.joc.9b02769](https://doi.org/10.1021/acs.joc.9b02769)



Three hole-transporting materials (HTMs) were prepared following a straightforward synthetic route by cross-linking arylamine-based ligands with a simple thieno[3,2-b]thiophene (TbT) core. The novel HTMs were fully characterized with standard techniques to gain insight into their optical and electrochemical properties and were incorporated in solution-processed mesoporous (FAPbI<sub>3</sub>)<sub>0.85</sub>(MAPbBr<sub>3</sub>)<sub>0.15</sub> perovskite-based solar cells. The similar molecular structure of the

synthesized HTMs was leveraged to investigate the role that the bridging units between the conjugated TbT core and the peripheral arylamine units plays on their properties and thereby on the photovoltaic response. A remarkable power conversion efficiency exceeding 18% was achieved for one of the TbT derivatives, which was slightly higher than the value measured for the benchmark spiro-OMeTAD.

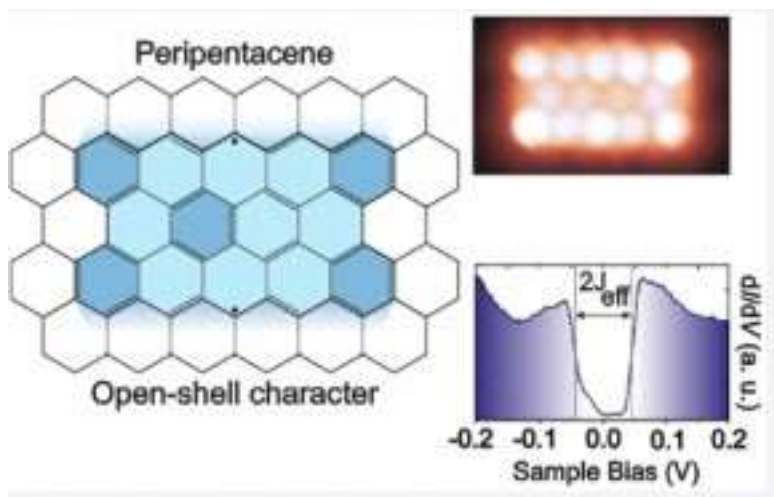
16) D. Alonso, D. Hernández-Castillo, L. Almagro, R. González-Alemán, D. Molero, Dolores; M. A. Herranz, E. Medina-Páez, J. Coro, R. Martínez-Álvarez, M. Suarez, N. Martín, "Diastereoselective Synthesis of Steroid-[60]Fullerene Hybrids and Theoretical Underpinning", *J. Org. Chem.* **2020**, *85*, 2426-2437 – doi: [10.1021/acs.joc.9b03121](https://doi.org/10.1021/acs.joc.9b03121)



The reaction of C<sub>60</sub> with pregnen-20-carboxaldehyde, a biologically active synthetic steroid, by using a 1,3-dipolar cycloaddition reaction (Prato's protocol) results in the formation of pyrrolidine rings bearing a new stereogenic center on the C2 of the five-membered ring. The formation of the fullerene-steroid hybrids proceeds with preference for the Re face of the 1,3-dipole, with formation of a diastereomeric mixture in 73:15 ratio. The investigation of the chiroptical properties of these conjugates allowed determining the absolute configuration of the new fulleropyrrolidines. In addition, a thorough spectroscopical study permitted to determine the structure of the two mono-cycloadducts. The electrochemical properties of the new hybrids were also evaluated by cyclic voltammetry, both systems exhibit three quasi-reversible reduction waves which are cathodically shifted in regard to the parent C<sub>60</sub>. Theoretical calculations help supporting the experimental data. A conformational study combining semiempirical methods and density functional theory has predicted the most stable diastereomer. On the basis of this agreement, a possible reaction mechanism is presented. Additionally, a molecular docking simulation has been carried out using the HIV-1 protease as receptor, thus paving the way to study the possible application of these stereoisomers in biomedicine.

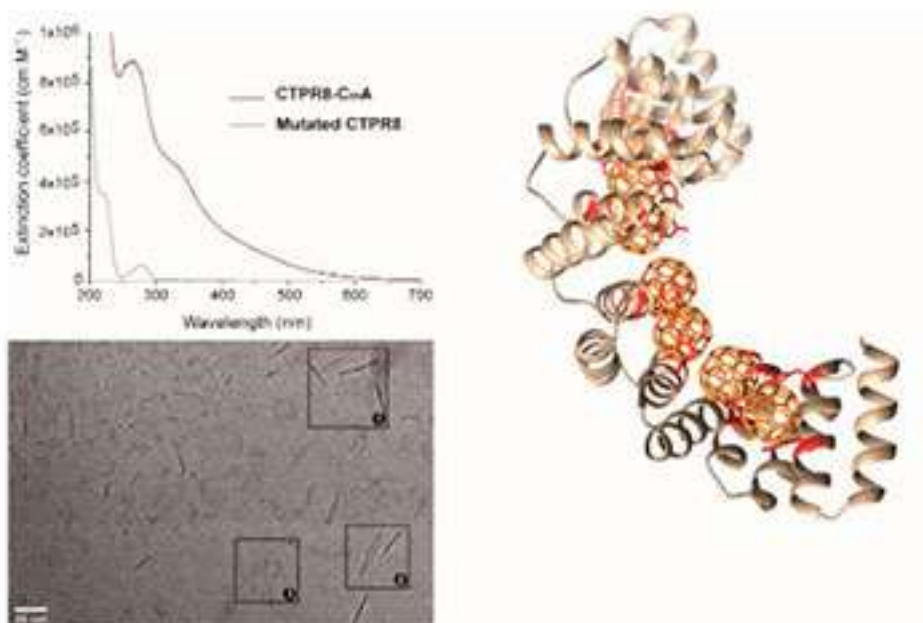
17) A. Sánchez-Grande, J. I. Urgel, L. Veis, S. Edalatmanesh, J. Santos, K. Lauwaet, P. Mutombo, J. M. Gallego, J. Brabec, P. Beran, D. Nachtigallová, R. Miranda, N. Martín, P. Jelínek, D. Ěcija, "Unravelling the Open-Shell Character of Peripentacene on Au(111)". *J. Phys. Chem. Lett.*, **2020**, in press. DOI : [dx.doi.org/10.1021/acs.jpcllett.0c02518](https://doi.org/10.1021/acs.jpcllett.0c02518).





Polycyclic aromatic hydrocarbons (PAHs) are a family of organic compounds comprising two or more fused aromatic rings which feature manifold applications in modern technology. Among these species, those presenting an open-shell magnetic ground state are of particular interest for organic electronic, spintronic, and non-linear optics and energy storage devices. Within PAHs, special attention has been devoted in recent years to the synthesis and study of the acene and fused acene (periacene) families, steered by their decreasing HOMO–LUMO gap with length and predicted open-shell character above some size. However, an experimental fingerprint of such magnetic ground state has remained elusive. Here, we report on the in-depth electronic characterization of isolated peripentacene molecules on a Au(111) surface. Scanning tunnelling spectroscopy, complemented by computational investigations, reveals an antiferromagnetic singlet ground state, characterized by singlet–triplet inelastic excitations with an experimental effective exchange coupling ( $J_{\text{eff}}$ ) of 40.5 meV. Our results deepen the fundamental understanding of organic compounds with magnetic ground states, featuring perspectives in carbon-based spintronic devices.

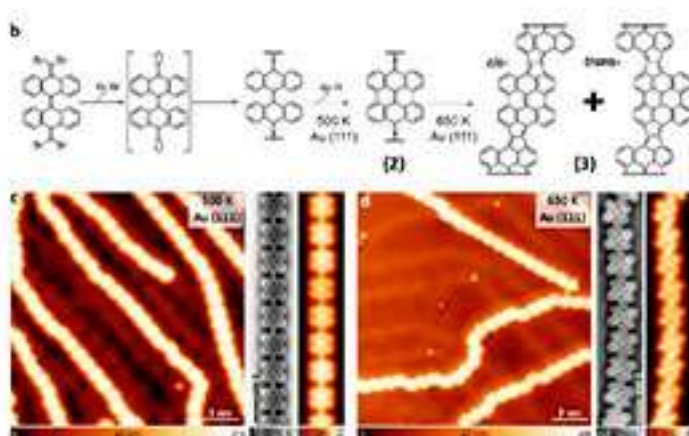
18) M. Liutkus, A. López-Andarias, S. H. Mejías, J. López-Andarias, D. Gil-Carton, F. Feixas, S. Osuna, W. Matsuda, T. Sakurai, S. Seki, C. Atienza, N. Martín, A. L. Cortajarena "Protein-directed crystalline 2D fullerene assemblies" *Nanoscale*, **2020**, *12*, 3614–3622 - doi: [10.1039/c9nr07083d](https://doi.org/10.1039/c9nr07083d)





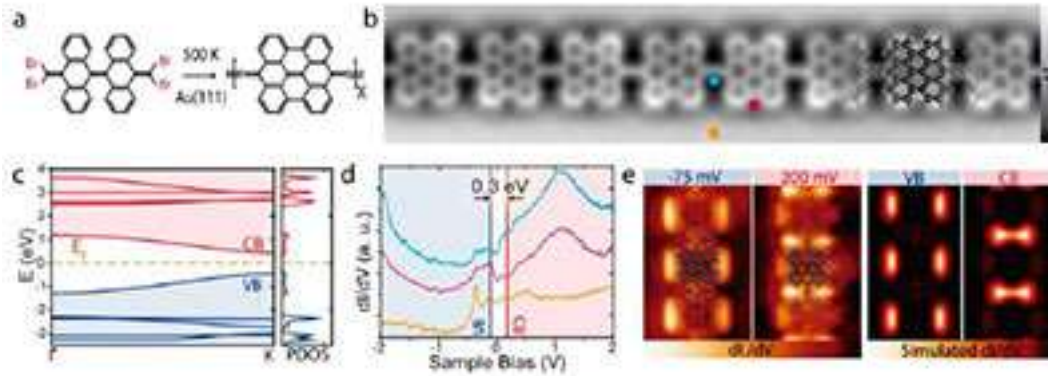
Water soluble 2D crystalline monolayers of fullerenes grow on planar assemblies of engineered consensus tetratricopeptide repeat proteins. Designed fullerene-coordinating tyrosine clamps on the protein introduce specific fullerene binding sites, which facilitate fullerene nucleation. Through reciprocal interactions between the components, the hybrid material assembles into two-dimensional 2 nm thick structures with crystalline order, that conduct photo-generated charges. Thus, the protein–fullerene hybrid material is a demonstration of the developments toward functional materials with protein-based precision control of functional elements.

19) B. de la Torre, A. Matěj, A. Sánchez-Grande, B. Cirera, B. Mallada, E. Rodríguez-Sánchez, J. Santos, J. I. Mendieta-Moreno, S. Edalatmanesh, K. Lauwaet, M. Otyepka, M. Medve, Á. Buendía, R. Miranda, N. Martín, P. Jelínek, D. Écija, "Tailoring p-conjugation and vibrational modes to steer on-surface synthesis of pentalene-bridged ladder polymers", *Nature Communications*, **2020**, 11:4567 - <https://doi.org/10.1038/s41467-020-18371-2>



The development of synthetic strategies to engineer n-conjugated polymers is of paramount importance in modern chemistry and materials science. Here we introduce a synthetic protocol based on the search for specific vibrational modes through an appropriate tailoring of the n-conjugation of the precursors, in order to increase the attempt frequency of a chemical reaction. First, we design a 1D n-conjugated polymer on Au(111), which is based on bisanthene monomers linked by cumulene bridges that tune specific vibrational modes. In a second step, upon further annealing, such vibrational modes steer the twofold cyclization reaction between adjacent bisanthene moieties, which gives rise to a long pentalene-bridged conjugated ladder polymer featuring a low bandgap. In addition, high resolution atomic force microscopy allows us to identify by atomistic insights the resonance form of the polymer, thus confirming the validity of the Glidewell and Lloyd's rules for aromaticity. This on-surface synthetic strategy may stimulate exploiting previously precluded reactions towards n-conjugated polymers with specific structures and properties.

20) B. Cirera, A. Sánchez-Grande, B. de la Torre, J. Santos, S. Edalatmanesh, E. Rodríguez-Sánchez, K. Lauwaet, B. Mallada-Faes, R. Zbořil, R. Miranda, O. Gröning, P. Jelínek, N. Martín, D. Écija, "Tailoring topological order and p-conjugation to engineer quasi-metallic polymers", *Nature Nanotechnology*, **2020**, 15, 437-443 - [doi: 10.1038/s41565-020-0668-7](https://doi.org/10.1038/s41565-020-0668-7)



Topological band theory predicts that a topological electronic phase transition between two insulators must proceed via closure of the electronic gap. Here, we use this transition to circumvent the instability of metallic phases in  $n$ -conjugated one-dimensional (1D) polymers. By means of density functional theory, tight-binding and GW calculations, we predict polymers near the topological transition from a trivial to a non-trivial quantum phase. We then use on-surface synthesis with custom-designed precursors to make polymers consisting of 1D linearly bridged acene moieties, which feature narrow bandgaps and in-gap zero-energy edge states when in the topologically non-trivial phase close to the topological transition point. We also reveal the fundamental connection between topological classes and resonant forms of 1D  $n$ -conjugated polymers.

## THESIS

TÍTULO: "Design and synthesis of organic p-type semiconductors: Toward efficient Perovskite Solar Cells"

DOCTORANDO: Javier Urieta Mora

UNIVERSIDAD: Complutense (Madrid)

FACULTAD/ESCUELA: Química

AÑO LECTURA: 27 de noviembre, 2020

CALIFICACIÓN: Sobresaliente "cum laude" por unanimidad



## LECTURES



Virtual 13<sup>th</sup> European School on Molecular Nanoscience

## ATTENDANCE CERTIFICATE

This is to certify that

**Nazario MARTÍN**

has attended the *Virtual 13th European School on Molecular Nanoscience (ESMolNa2020)* celebrated online from June 3<sup>rd</sup> to 5<sup>th</sup> 2020 and has presented an Invited lecture entitled:

*Bottom-up Synthesis of (Chiral) Nanographenes*

Valencia (Spain)  
June 5<sup>th</sup> 2020



Eugenio Coronado  
Chairman

