

# Currículum vitae

Nombre: M. Carmen Ruiz Delgado

Fecha: 27-09-2016

## PERSONAL DATA

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Family name: Ruiz Delgado  
ID/Passport no: 77469096-J  
Nationality: Spain

Forename: M<sup>a</sup> del Carmen  
Date of birth : May 7, 1977  
Gender: Female

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## PRESENT PROFESSIONAL POSITION

Institution: University of Málaga  
Faculty, School or Institute: Faculty of Science  
Department: Department of Physical Chemistry  
Address: Campus de Teatinos  
Post Cod: 29071 Province: Málaga  
Country: Spain

Telephone (indicate prefix, number and extension): 952-131863  
Fax: -  
E-mail: carmenrd@uma.es

Field of study (UNESCO codes): Main Field: 23; Subfields: 2306.10, 2211.09, 2210.20, 2206.08, 2206.09, 2206.10, 2209.14, 3312.08

Professional status: Ramón y Cajal Research Fellow

Start date: November 19, 2010

### Administrative status

Permanent Staff       Hired on contracts       Acting     

Fellowship holder  
 Others specify:

Full-time   
Part-time

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## PRESENT RESEARCH AREA

Brief summary (key words).

Conjugated Organic Materials, Electronic Devices, Organic Semiconductors, Molecular Spectroscopy (UV-Vis, IR, Raman, UPS), Thermospectroscopy, Spectroelectrochemistry, Charge-transport, Non Linear Optics, Quantum-chemical Calculations (DFT, HF, semi-empirical), Molecular Dynamics (MD), Hybrid QM/MM methods.

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## ACADEMIC BACKGROUND

Bachelor	Centre	Date
Chemical Engineering	University of Málaga	04/04/2001

<i>Ph.D.</i>	<i>Centre</i>	<i>Thesis Supervisor</i>	<i>Date</i>
<i>Doctor</i>	<i>University of Málaga</i>	<i>Prof. Dr. Juan Teodomiro Navarrete</i> <i>Prof. Dr. Víctor Hernández Jolín</i> <i>Prof. Dr. Juan Casado Cordón</i>	<i>27/06/2006</i>

### PAST SCIENTIFIC EXPERIENCE (\*)

<i>Position</i>	<i>R&amp;D Centre</i>	<i>Institution (**)</i>	<i>Start date</i>	<i>End date</i>
<i>Post-Bachelor Research Fellow (MEC)</i>	<i>Department of Chemical Engineering</i>	<i>University of Málaga</i>	<i>01/09/1999</i>	<i>31/08/2000</i>
<i>Research Fellow (FQM-0159)</i>	<i>Department of Physical Chemistry</i>	<i>University of Málaga</i>	<i>01/05/2002</i>	<i>31/12/2002</i>
<i>FPU Research Fellow (MEC)</i>	<i>Department of Physical Chemistry</i>	<i>University of Málaga</i>	<i>01/01/2003</i>	<i>31/12/2006</i>
<i>Research Associate</i>	<i>Department of Physical Chemistry</i>	<i>University of Málaga</i>	<i>12/02/2007</i>	<i>23/03/2007</i>
<i>Visiting Postdoctoral Scholar (UMA Research Fellow)</i>	<i>Institute of Materials Science of Aragón</i>	<i>University of Zaragoza (Spain)</i>	<i>15/01/2007</i>	<i>23/03/2007</i>
<i>Postdoctoral Fellow (MEC/Fulbright)</i>	<i>School of Chemistry and Biochemistry</i>	<i>Georgia Institute of Technology (USA)</i>	<i>01/04/2007</i>	<i>31/03/2009</i>
<i>Postdoctoral Research Fellow</i>	<i>School of Chemistry and Biochemistry</i>	<i>Georgia Institute of Technology (USA)</i>	<i>01/04/2009</i>	<i>31/03/2010</i>
<i>Postdoctoral Research Fellow</i>	<i>Department of Physical Chemistry</i>	<i>University of Málaga</i>	<i>08/04/2010</i>	<i>18/11/2010</i>
<i>Ramón y Cajal Researcher</i>	<i>Department of Physical Chemistry</i>	<i>University of Málaga</i>	<i>19/11/2010</i>	<i>-</i>

(\*) The information contained in this chart will be used to verify the placement requirements, according to the Call.

(\*\*) If the Institution is a "joint centre", you should specify all the centres involved in running it.

### LANGUAGES (N = NORMAL, G = GOOD, P = PERFECTLY)

<i>Language</i>	<i>Speaking</i>	<i>Reading</i>	<i>Writing</i>
<i>English</i>	<i>G</i>	<i>P</i>	<i>P</i>
<i>German</i>	<i>N</i>	<i>N</i>	<i>N</i>

## PARTICIPATION IN RESEARCH PROJECTS

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*PROJECT TITLE: Spectroscopic, Electrochemical, Spectroelectrochemical, and Quantum-Chemical DFT Study of Molecular Materials for Molecular Electronic.*

*FINANCIAL ENTITY: Proyecto DGI BQU2003-3194*

*LENGHT FROM:01/12/2003 TO: 30/11/2006*

*PRINCIPAL INVESTIGATOR: Prof. Dr. Juan Teodomiro López Navarrete*

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*PROJECT TITLE: Poly-conjugated Molecules for Molecular Electronics and Photonics: Establishment of Structure-Properties relationships using Spectroscopical and Spectroelectrochemical Techniques.*

*FINANCIAL ENTITY: Proyecto coordinado DGI (MEC) CTQ2006-14987-C02-01*

*LENGHT FROM:01/10/2006 TO: 30/09/2009*

*PRINCIPAL INVESTIGATOR: Prof. Dr. Juan Teodomiro López Navarrete*

**Total amount:** 88.088 euros

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*PROJECT TITLE: Materials for Molecular Electronics and Photonics: Design and Characterization of nanostructured biosensors*

*FINANCIAL ENTITY: Proyecto de Investigación de Excelencia (Junta de Andalucía). P06-FQM-01678*

*LENGHT FROM:01/02/2007 TO: 31/01/2010*

*PRINCIPAL INVESTIGATOR: Prof. Dr. Juan Teodomiro López Navarrete*

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*PROJECT TITLE: Novel Poly-conjugated Materials for Molecular Electronics and Photonics: Study of Intra- and Inter-molecular Optoelectronic Properties by Spectroscopic Techniques and Quantum-Chemical calculations*

*FINANCIAL ENTITY: Proyecto del Plan Nacional de I+D+I (MCINN) CTQ2009-10098*

*LENGHT FROM: 01/10/2009 TO: 30/09/2012*

*PRINCIPAL INVESTIGATOR: Prof. Dr. Juan Teodomiro López Navarrete*

**Total amount:** 356.950 euros

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*PROJECT TITLE: Materials for Molecular Electronics and Photonics: Fabrication and Characterization of Organic Field-Effect Transistors (OFETs)*

*FINANCIAL ENTITY: Proyecto de Investigación de Excelencia (Junta de Andalucía). P06-FQM-0478*

*LENGHT FROM:01/02/2010 TO: 31/01/2014*

*PRINCIPAL INVESTIGATOR: Prof. Dr. Juan Teodomiro López Navarrete*

**Total amount:** 207.923,68 euros

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*PROJECT TITLE: Estudio Espectroscópico y Teórico de Materiales Orgánicos para Electrónica Orgánica*

*FINANCIAL ENTITY: Proyecto del Plan Nacional de I+D+I (MCINN) CTQ2012-33733*

*LENGHT FROM: 01/01/2013 TO: 31/12/2015*

PRINCIPAL INVESTIGATOR: Prof. Dr. Juan Teodomiro López Navarrete  
Total amount: 284.310 euros

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PROJECT TITLE: *Organic Optoelectronic Interfaces (IRG-2)*

FINANCIAL ENTITY: *University of Minnesota, Materials Research Science and Engineering Center (MRSEC) Program of the National Science Foundation (NSF) under Award DMR-0212302 and DMR-0819885.*

LENGHT FROM:01/04/2007 TO: 31/03/2010

PRINCIPAL INVESTIGATOR: *Prof. Dr. C. D. Frisbie and Prof. Dr. Jean-Luc Brédas.*

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PROJECT TITLE: *Ramon y Cajal Research Contract (RYC-2010-07186)*

FINANCIAL ENTITY: *Ministerio de Ciencia e Innovación*

LENGHT FROM: 19/11/2010 TO: 18/11/2015

Funding: 192.480,00 euros

PRINCIPAL INVESTIGATOR: *Dr. María del Carmen Ruiz Delgado*

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*Junta de Andalucía Research Grants:*

*\* The Research Excellence Junta de Andalucía Program Award Grants to support research groups.*

*Member of the Biopolymers and Conductive Polymers (Código FQM-0159) research group of excellence.*

*Convocatoria 2002: 31.216,00 €. (Mark: 25/25). Research Group of Excellence.*

*Convocatoria 2003: 12.045,67 €. (Mark: 25/25). Research Group of Excellence.*

*Convocatoria 2004: 10.411,23 €. (Mark: 25/25). Research Group of Excellence.*

*Convocatoria 2005: 12.505,43 €. (Mark: 32/32). Research Group of Excellence.*

*Convocatoria 2006: 9.691,65 €. (Mark: 32/32). Research Group of Excellence.*

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## PUBLICATIONS

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Indicate volume, first and last page (year) and Key.

Key: B= full book, CB.= chapter of book, A= article, R= review, E= editor

(\*) Those publications in process and not yet published, just specify publication status. (\*\*) Optionally specify the most important aspects of each publication to assess quality (e.g. journal impact index, journal position on lists of the corresponding fields, cites received or other repercussion indicators)

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*AUTHORS (in order of authorship): C. Moreno Castro, M.C. Ruiz Delgado, V. Hernández, S. Hotta, J. Casado and J. T. López Navarrete.*

*TITLE: Efficiency of the  $\pi$ -Conjugation in a novel Family of  $\alpha,\alpha$ -bisphenyl end-capped oligothiophenes by Means of Raman Spectroscopy*

*JOURNAL/BOOK TITLE: J. Chem. Phys. 116, 10419-10427 (2002) KEY: A*

*DATE OF PUBLICATION (\*): 2002*

*MOST OUTSTANDING ASPECTS (\*\*): Journal impact index (JCR 2008): 3.149; journal position on list of "Physics, atomic, molecular & chemical": 5/31; cites received: 40 (isi web of knowledge)*

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*AUTHORS (in order of authorship): C. Moreno Castro, M.C. Ruiz Delgado, V. Hernández, Y. Shirota, J. Casado and J. T. López Navarrete.*

*TITLE: Vibrational Spectroscopy Features of a Novel Family of Amorphous Molecular Materials Containing an oligothiophene Moiety as Colour-Tunable Emitting Materials.*

*JOURNAL/BOOK TITLE: J. Phys. Chem. B, 106, 7163-7170 (2002). KEY: A*

*DATE OF PUBLICATION (\*): 2002*

*MOST OUTSTANDING ASPECTS (\*\*): Journal impact index (JCR 2008): 4.189; journal position on list of "Chemistry, Physical": 22/113; cites received: 32 (isi web of knowledge)*

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*AUTHORS (in order of authorship): J. Casado, R.G. Hicks, V. Hernández, D.J.T. Myles, M. C. Ruiz Delgado and J. T. López Navarrete.*

*TITLE: Infrared and Raman Features of a Series of  $\alpha,\omega$ -bis(arylthio)oligothiophenes as molecular wires. A  $\pi$ -electron delocalization efficiency study.*

*JOURNAL/BOOK TITLE: J. Chem. Phys. 118, 1912-1920 (2003). KEY: A*

*DATE OF PUBLICATION (\*): 2003*

*MOST OUTSTANDING ASPECTS (\*\*): Journal impact index (JCR 2008): 3.149; journal position on list of "Physics, atomic, molecular & chemical": 5/31; cites received: 10 (isi web of knowledge)*

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*AUTHORS (in order of authorship): J. Casado, M.C. Ruiz Delgado, Y. Shirota, V. Hernández and J. T. López Navarrete.*

*TITLE: Computation and Spectroelectrochemistry as Complementary Tools for the Study of Electrochemically Induced Charged Defects in 4-[Bis(4-methylphenyl)amino]phenyl Oligothiophenes as Model Systems for Hole-Transporting Materials.*

*JOURNAL/BOOK TITLE: J. Phys. Chem. B 107, 2637-2644 (2003). KEY: A*

*DATE OF PUBLICATION (\*): 2003*

MOST OUTSTANDING ASPECTS (\*\*): *Journal impact index (JCR 2008): 4.189; journal position on list of "Chemistry,Physical": 22/113; cites received: 29 (isi web of knowledgege)*

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AUTHORS (in order of authorship): **M. C. Ruiz Delgado**, V. Hernández, J. Casado, J. T. López Navarrete, J.-M. Raimundo, P. Blanchard and J. Roncali.

TITLE: *Vibrational and Quantum-Chemical Study of Push-Pull Chromophores for Second Order Nonlinear Optics Derived from Rigidified Thiophene-Based- $\pi$ -Conjugating Spacers.*

JOURNAL/BOOK TITLE: Chem. Eur. J. 9, 3670-3682 (2003).

KEY: A

DATE OF PUBLICATION (\*): 2003

MOST OUTSTANDING ASPECTS (\*\*): *Journal impact index (JCR 2008): 5.484; journal position on list of "Chemistry, Multidisciplinary": 12/127; cites received: 24 (isi web of knowledgege)*

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AUTHORS (in order of authorship): **M. C. Ruiz Delgado**, V. Hernández, J. T. López Navarrete, S. Tanaka and Y. Yamashita.

TITLE: *Combined Spectroscopic and Theoretical Study of Narrow-Bandgap Heterocyclic Oligomers Containing Alternating Aromatic-Donor and o-Quinoid-Acceptor Units.*

JOURNAL/BOOK TITLE: J. Phys. Chem. B. 108 (8), 2516-2526 (2004). KEY: A

DATE OF PUBLICATION (\*): 2004

MOST OUTSTANDING ASPECTS (\*\*): *Journal impact index (JCR 2008): 4.189; journal position on list of "Chemistry,Physical": 22/113; cites received: 24 (isi web of knowledgege)*

---

AUTHORS (in order of authorship): **M. C. Ruiz Delgado**, J. Casado, V. Hernández, J. T. López Navarrete, G. Fuhrmann and P. Bäuerle.

TITLE: *Combined Raman and Computational Study of a Novel Series of Macrocyclic  $\pi$ -Conjugated Diacetylene-Bridged  $\alpha$ -linked Oligothiophenes.*

JOURNAL/BOOK TITLE: J. Phys. Chem. B 108, 3158-3167 (2004). KEY: A

DATE OF PUBLICATION (\*): 2004

MOST OUTSTANDING ASPECTS (\*\*): *Journal impact index (JCR 2008): 4.189; journal position on list of "Chemistry,Physical": 22/113; cites received: 22 (isi web of knowledgege)*

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AUTHORS (in order of authorship): J. Casado, V. Hernández, R. Ponce Ortiz, M.C. Ruiz Delgado, J. T. López Navarrete, G. Fuhrmann and P. Bäuerle.

TITLE: *Application of Raman Spectroscopy and Quantum-Chemistry for Featuring the Structure of Positively Charged Species in Macrocyclic  $\pi$ -Conjugated Diacetylene-Bridged Oligothiophenes.*

JOURNAL/BOOK TITLE: J. Raman Spectrosc. 35, 592-599 (2004).

KEY: A

DATE OF PUBLICATION (\*): 2004

MOST OUTSTANDING ASPECTS (\*\*): *Journal impact index (JCR 2008): 3.526; journal position on list of "Spectroscopy": 6/39; cites received: 16 (isi web of knowledgege)*

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AUTHORS (in order of authorship): J. Casado, V. Hernández, O.-K. Kim, J.-M. Lehn, J. T. López Navarrete, S. Delgado Ledesma, R. Ponce Ortiz, M.C. Ruiz Delgado, Y. Vida, E. Pérez-Inestrosa.

TITLE: *Vibrational and Quantum-Chemical study of nonlinear optical chromophores containing dithienothiophene as the electron relay. .*

JOURNAL/BOOK TITLE: Chem. Eur. Journal, 10, 3805-3816 (2004). KEY: A

DATE OF PUBLICATION (\*): 2004

MOST OUTSTANDING ASPECTS (\*\*): *Journal impact index (JCR 2008): 5.484; journal position on list of "Chemistry, Multidisciplinary": 12/127; cites received: 23 (isi web of knowledge)*

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AUTHORS (in order of authorship): R. Ponce Ortiz, M.C. Ruiz Delgado, J. Casado, V. Hernández, O.-K. Kim, H. Y. Woo, J.T. López Navarrete.

TITLE: *Electronic modulation of dithienothiophene (DTT) as  $\pi$ -center of D- $\pi$ -D chromophores on optical and redox properties: Analysis by UV-Vis-NIR and Raman spectroscopies combined with electrochemistry and quantum chemical DFT calculations.*

JOURNAL/BOOK TITLE: J. Am. Chem. Soc. 126, 13363-13376 (2004). KEY: A

DATE OF PUBLICATION (\*): 2004

MOST OUTSTANDING ASPECTS (\*\*): *Journal impact index (JCR 2008): 8.091; journal position on list of "Chemistry, Multidisciplinary": 7/127; cites received: 19 (isi web of knowledge)*

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AUTHORS (in order of authorship): J. Casado, R. Ponce Ortiz, M.C. Ruiz Delgado, V. Hernández, J.T. López Navarrete, P. Blanchard, M. Allain, J. Roncalí.

TITLE: *Alternated Quinoid/Aromatic Units in Terthiophenes Building Blocks for Electroactive Narrow Band Gap Polymers. Extended Spectroscopic, Solid State, Electrochemical, and Theoretical Study.*

JOURNAL/BOOK TITLE: J. Phys. Chem. B. 109(35), 16616-16627 (2005). KEY: A

DATE OF PUBLICATION (\*): 2005

MOST OUTSTANDING ASPECTS (\*\*): *Journal impact index (JCR 2008): 4.189; journal position on list of "Chemistry, Physical": 22/113; cites received: 19 (isi web of knowledge)*

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AUTHORS (in order of authorship): J. Casado, R. Ponce Ortiz, M. C. Ruiz Delgado, R. Azumi, R. T. Oakley, V. Hernández, J.T. López Navarrete.

TITLE: *Multidisciplinary Physicochemical Analysis of Oligothiophenes End-Capped by Nitriles: Electrochemistry, UV-Vis-NIR, IR, and Raman Spectroscopies and Quantum Chemistry*

JOURNAL/BOOK TITLE: J. Phys. Chem. B, 109 (20), 10115-10125 (2005) KEY: A

DATE OF PUBLICATION (\*): 2005

MOST OUTSTANDING ASPECTS (\*\*): *Journal impact index (JCR 2008): 4.189; journal position on list of "Chemistry, Physical": 22/113; cites received: 18 (isi web of knowledge)*

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AUTHORS (in order of authorship): R. Andreu, M. J. Blesa, L. Carrasquer, J. Garin, J. Orduna, B. Villacampa, R. Alcalá, J. Casado, M. C. Ruiz Delgado, J. T. Lopez Navarrete, M. Allain.

TITLE: *Tuning First Molecular Hyperpolarizabilities through the Use of Proaromatic Spacers.*

JOURNAL/BOOK TITLE: J. Am. Chem. Soc. 127(24), 8835-8845 (2005). KEY: A

DATE OF PUBLICATION (\*): 2005

MOST OUTSTANDING ASPECTS (\*\*): *Journal impact index (JCR 2008): 8.091; journal position on list of "Chemistry, Multidisciplinary": 7/127; cites received: 40 (isi web of knowledge)*

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*AUTHORS (in order of authorship): J. Casado, V. Hernandez, M. C. Ruiz Delgado, R. P. Ortiz, J. T. Lopez Navarrete, A. Facchetti, T. J. Marks.*

*TITLE: Incisive Structure-Spectroscopic Correlation in Oligothiophenes Functionalized with ( $\pm$ ) Inductive/Mesomeric Fluorine Groups: Joint Raman and DFT Study.*

*JOURNAL/BOOK TITLE: J. Am. Chem. Soc. 127(38); 13364-13372 (2005) KEY: A*

*DATE OF PUBLICATION (\*): 2005*

*MOST OUTSTANDING ASPECTS (\*\*): Journal impact index (JCR 2008): 8.091; journal position on list of "Chemistry, Multidisciplinary": 7/127; cites received: 6 (isi web of knowledge)*

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*AUTHORS (in order of authorship): A. Berlin, S. Grimoldi, G. Zotti, R. Malavé Osuna, M. C. Ruiz Delgado, R. Ponce Ortiz, V. Hernández, J. T. López Navarrete.*

*TITLE: Synthesis and Characterization of a Novel Terthiophene-Based Quinodimethane Bearing a 3,4-Ethylenedioxythiophene Central Unit.*

*JOURNAL/BOOK TITLE: J. Phys. Chem. B., 109, 22308-22318 (2005). KEY: A*

*DATE OF PUBLICATION (\*): 2005*

*MOST OUTSTANDING ASPECTS (\*\*): Journal impact index (JCR 2008): 4.189; journal position on list of "Chemistry, Physical": 22/113; cites received: 3 (isi web of knowledge)*

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*AUTHORS (in order of authorship): R. Malavé Osuna, R. Ponce Ortiz, M. C. Ruiz Delgado, Y. Sakamoto, T. Suzuki, V. Hernández, J. T. López Navarrete.*

*TITLE: Synthesis and Characterization of three novel perfluoro-oligothiophenes ranging in length from the trimer to the pentamer.*

*JOURNAL/BOOK TITLE: J. Phys. Chem. B., 109, 20737-20745 (2005). KEY: A*

*DATE OF PUBLICATION (\*): 2005*

*MOST OUTSTANDING ASPECTS (\*\*): Journal impact index (JCR 2008): 4.189; journal position on list of "Chemistry, Physical": 22/113; cites received: 6 (isi web of knowledge)*

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*AUTHORS (in order of authorship): J. Casado, M. Z. Zgierski, R. G. Hicks, D. J.T. Myles, P. M. Viruela, E. Ortí, M.C. Ruiz Delgado, V. Hernández, J.T. López Navarrete.*

*TITLE: pMesitylthio-oligothiophenes in various redox states. Molecular and electronic views as offered by spectroscopy and theory.*

*JOURNAL/BOOK TITLE: J. Phys. Chem. A., 109, 11275-11284 (2005). KEY: A*

*DATE OF PUBLICATION (\*): 2005*

*MOST OUTSTANDING ASPECTS (\*\*): Journal impact index (JCR 2008): 2.871; journal position on list of "Physics, atomic, molecular & chemical": 7/31; cites received: 5 (isi web of knowledge)*

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*AUTHORS (in order of authorship): J. Casado, M.C. Ruiz Delgado, M.C. Rey Merchán, V. Hernández, J.T. López Navarrete, T. Pappenfus, N. Williams, W. J. Stegner, J. C. Jonson, B. A. Edlund, D. E. Janzen, K. R. Mann, J. Orduna, B. Villacampa.*

*TITLE: Optical, Redox and NLO Properties of Tricyanovinyl Oligothiophenes. Comparisons Between the Symmetric and Asymmetric Substitution Patterns.*

*JOURNAL/BOOK TITLE: Chem. Eur. Journal, 12, 5458-5470 (2006). KEY: A*

*DATE OF PUBLICATION (\*): 2006*

*MOST OUTSTANDING ASPECTS (\*\*): Journal impact index (JCR 2008): 5.484; journal position on list of "Chemistry, Multidisciplinary": 12/127; cites received: 11 (isi web of knowledge)*

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*AUTHORS (in order of authorship): J. Casado, M. Moreno Oliva, M. C. Ruiz Delgado, R. Ponce Ortiz, J. J. Quirante, J. T. López Navarrete, K. Takimiya, T. Otsubo.*

*TITLE: Hybrid organic semiconductors including chalcogen atoms in  $\pi$ -conjugated skeletons. Tuning of optical, redox, and vibrational properties by heavy atom conjugation.*

*JOURNAL/BOOK TITLE: J. Phys. Chem. A, 110, 7422-7430 (2006). KEY: A*

*DATE OF PUBLICATION (\*): 2006*

*MOST OUTSTANDING ASPECTS (\*\*): Journal impact index (JCR 2008): 2.871; journal position on list of "Physics, atomic, molecular & chemical": 7/31; cites received: 3 (isi web of knowledge)*

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*AUTHORS (in order of authorship): A. Schmidt, A. Lindner, M. Nieger, M. C. Ruiz Delgado, F. J. Ramírez.*

*TITLE: Syntheses,  $\pi$ -stacking interactions, and base-pairings of uracil-pyridinium salts and uracilyl-betaines with nucleobases.*

*JOURNAL/BOOK TITLE: Org. Biomol. Chem., 16, 3056-3066 (2006) KEY: A*

*DATE OF PUBLICATION (\*): 2006*

*MOST OUTSTANDING ASPECTS (\*\*): Journal impact index (JCR 2007): 3.550; journal position on list of "Chemistry, Organic": 10/55; cites received: 9 (isi web of knowledge)*

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*AUTHORS (in order of authorship): J. Casado, M. Moreno Oliva, M. C. Ruiz Delgado, J. T. López Navarrete, L. Sánchez, N. Martín, R. Andréu, L. Carrasquer, J. Garín, J. Orduna.*

*TITLE: Vibrational Fingerprint of the Structural Tuning in Push-Pull Organic Chromophores with Quinoid or Pro-Aromatic Spacers.*

*JOURNAL/BOOK TITLE: J. Chem. Phys. 126, 074701-1/074701-8 (2007). KEY: A*

*DATE OF PUBLICATION (\*): 2007*

*MOST OUTSTANDING ASPECTS (\*\*): Journal impact index (JCR 2008): 3.149; journal position on list of "Physics, atomic, molecular & chemical": 5/31.*

---

*AUTHORS (in order of authorship): R. Malavé Osuna, R. Ponce Ortiz, M. C. Ruiz Delgado, V. G. Nenajdenko, V. V. Sumerin, E. S. Balenkova, V. Hernández, J. T. López Navarrete.*

*TITLE: Fourier Transform Raman and DFT Study of Three Annulated Oligothiophenes with Different Molecular Shapes.*

*JOURNAL/BOOK TITLE: ChemPhysChem 8, 745-750 (2007). KEY: A*

*DATE OF PUBLICATION (\*): 2007*

*MOST OUTSTANDING ASPECTS (\*\*): Journal impact index (JCR 2008): 3.636; journal position on list of "Physics, atomic, molecular & chemical": 3/31; cites received: 3 (isi web of knowledge)*

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*AUTHORS (in order of authorship): J. Casado, Marek Z. Zgierski, M. C. Ruiz Delgado, J. T. López Navarrete, M. Mas-Torrent, C. Rovira.*

*TITLE: Tetrathiafulvalene-Based Materials for OFETs. Inspection of their Semiconductor Properties by Means of Molecular Spectroscopy and Quantum Chemistry.*

*JOURNAL/BOOK TITLE: J. Phys. Chem. C, 111, 10110-10118 (2007). KEY: A*

*DATE OF PUBLICATION (\*): 2007*

*MOST OUTSTANDING ASPECTS (\*\*): Journal impact index (JCR 2008): 3.396; journal position on list of "Materials Science, Multidisciplinary": 26/192; cites received: 7 (isi web of knowledge)*

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*AUTHORS (in order of authorship): M. Carmen Ruiz Delgado, J. Orduna, M. Moreno Oliva, J. Casado, and J. T. López Navarrete.*

*TITLE: Theoretical understanding of the increment of  $\beta$  upon protonation of pyridine peripheral octupolar molecules: Toward nonlinear optical sensor.*

*JOURNAL/BOOK TITLE: J. Chem. Phys., 127, 164704-1/164704-6 (2007). KEY: A*

*DATE OF PUBLICATION (\*): 2007*

*MOST OUTSTANDING ASPECTS (\*\*): Journal impact index (JCR 2008): 3.149; journal position on list of "Physics, atomic, molecular & chemical": 5/31; cites received: 2 (isi web of knowledge)*

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*AUTHORS (in order of authorship): M. Moreno Oliva, J. Casado, J. T. López Navarrete, G. Henrich, M. Carmen Ruiz Delgado, J. Orduna.*

*TITLE: Linear and Nonlinear Optical Properties of Pyridine-Based Octopolar Chromophores Designed for Chemical Sensing. Joint Spectroscopic and Theoretical Study.*

*JOURNAL/BOOK TITLE: J. Phys. Chem. C, 111, 18778-18784 (2007). KEY: A*

*DATE OF PUBLICATION (\*): 2007*

*MOST OUTSTANDING ASPECTS (\*\*): Journal impact index (JCR 2008): 3.396; journal position on list of "Materials Science, Multidisciplinary": 26/192; cites received: 7 (isi web of knowledge)*

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*AUTHORS (in order of authorship): M. Carmen Ruiz Delgado, J. Casado, V. Hernández, J.T. López Navarrete, J. Orduna, B. Villacampa, R. Alicante, J.-M. Raimundo, P. Blanchard, J. Roncali.*

*TITLE: Electronic, Optical, and Vibrational Properties of Bridged Dithienylethylene-Based NLO Chromophores.*

*JOURNAL/BOOK TITLE: J. Phys. Chem. C, 112, 3109-3120 (2008). KEY: A*

*DATE OF PUBLICATION (\*): 2008*

MOST OUTSTANDING ASPECTS (\*\*): *Journal impact index (JCR 2008): 3.396; journal position on list of "Materials Science, Multidisciplinary": 26/192; cites received: 3 (isi web of knowledage)*

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AUTHORS (in order of authorship): J. Casado, S. R. González, M. C. Ruiz Delgado, M. Moreno Oliva, J. T. López Navarrete, R. Caballero, P. de la Cruz, F. Langa.

TITLE: *Ferrocenyl-Ended Thieno-Vinylene Oligomers: Donor-Acceptor Polarization and Mixed Valence Properties with Emphasis on the Raman Mapping of Localized-to-Delocalized Transitions.*

JOURNAL/BOOK TITLE: Chem. Eur. Journal 151, 2548-2559 (2009) KEY: A

DATE OF PUBLICATION (\*): 2009

MOST OUTSTANDING ASPECTS (\*\*): *Journal impact index (JCR 2008): 5.484; journal position on list of "Chemistry, Multidisciplinary": 12/127.*

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AUTHORS (in order of authorship): . Malavé Osuna, M.C. Ruiz Delgado; V. Hernández; J. T. López Navarrete; B. Vercelli; G. Zotti; J. J. Novoa; Y. Suzuki; S. Yamaguchi; JJ. T. Henssler; Adam J. Matzger.

TITLE: *Oxidation of End-Capped Pentathienoacenes and Characterization of Their Radical Cations.*

JOURNAL/BOOK TITLE: Chem. Eur. Journal 15, 12346-12361 (2009) KEY: A

DATE OF PUBLICATION (\*): 2009

MOST OUTSTANDING ASPECTS (\*\*): *Journal impact index (JCR 2008): 5.484; journal position on list of "Chemistry, Multidisciplinary": 12/127.*

---

AUTHORS (in order of authorship): M. Moreno Oliva; J. Casado; J. T. López Navarrete; G. Hennrich; S. van Cleuvenbergen; I. Asselberghs; K. Clays; M.C. Ruiz Delgado; J.L. Brédas; J. Sérgio Seixas de Melo; L. de Cola.

TITLE: *Synthesis, Spectroscopy, Nonlinear Optics and Theoretical Investigations of Thienylethynyl Octopoles with Tunable Core.*

JOURNAL/BOOK TITLE: Chem. Eur. Journal 15, 8223-8234 (2009) KEY: A

DATE OF PUBLICATION (\*): 2009

MOST OUTSTANDING ASPECTS (\*\*): *Journal impact index (JCR 2008): 5.484; journal position on list of "Chemistry, Multidisciplinary": 12/127.*

---

AUTHORS (in order of authorship): N. Martinelli; Y. Olivier; S. Athanasopoulos; M.C. Ruiz Delgado; K. R. Pigg; D.A. da Silva Filho; R.S. Sánchez-Carrera; E. Venuti; R. G. Della Valle; J.L. Brédas; D. Beljonne; J. Cornil

TITLE: *Influence of Intermolecular Vibrations on the Electronic Coupling in Organic Semiconductors: The case of Anthracene and Perfluoropentacene.*

JOURNAL/BOOK TITLE: ChemPhysChem. 10, 2265-2273 (2009) KEY: A

DATE OF PUBLICATION (\*): 2009

MOST OUTSTANDING ASPECTS (\*\*): *Inside Cover of Vol. 13, ChemPhysChem 2009.*

*Journal impact index (JCR 2008): 3.636; journal position on list of "Physics, atomic, molecular & chemical": 3/31.*

---

*AUTHORS (in order of authorship): S. Salman, M.C. Ruiz Delgado\*, V. Coropceanu, J.L. Brédas.*

*TITLE: Electronic Structure and Charge-Transport Parameters of Functionalized Tetracene Crystals: Impact of Partial Fluorination and Alkyl or Alkoxy Derivatization.*

*JOURNAL/BOOK TITLE: Chemistry of Materials 21, 3593-3601 (2009) KEY: A*

*DATE OF PUBLICATION (\*): 2009*

*MOST OUTSTANDING ASPECTS (\*\*): Journal impact index (JCR 2008): 5.046; journal position on list of "Materials Science, Multidisciplinary": 14/192.*

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*AUTHORS (in order of authorship): M.C. Ruiz Delgado, K. R. Pigg, D.A. da Silva Filho, N. E. Gruhn, Y. Sakamoto, T. Suzuki, R. Malave, J. Casado, V. Hernández, J.T. López Navarrete, N. G. Martinelli, J. Cornil, R.S. Sánchez-Carrera, V. Coropceanu, J.L. Brédas.*

*TITLE: Impact of Perfluorination on the Charge-Transport Parameters of Oligoacene Crystals.*

*JOURNAL/BOOK TITLE: J. Am. Chem. Soc. 131, 1502-1512 (2009)*

*KEY: A*

*DATE OF PUBLICATION (\*): 2009*

*MOST OUTSTANDING ASPECTS (\*\*): Journal impact index (JCR 2008): 8.091; journal position on list of "Chemistry, Multidisciplinary": 7/127.*

---

*AUTHORS (in order of authorship): M.C. Ruiz Delgado, E.G. Kim, D.A. da Silva Filho, J.L. Brédas.*

*TITLE: Tuning the Charge-Transport Parameters of Perylene Diimide Single Crystals via End and/or Core Functionalization: A Density Functional Theory Investigation.*

*JOURNAL/BOOK TITLE: J. Am. Chem. Soc. 132, 3375-3387 (2010) KEY: A*

*DATE OF PUBLICATION (\*): 2010*

*MOST OUTSTANDING ASPECTS (\*\*): Journal impact index (JCR 2008): 8.091; journal position on list of "Chemistry, Multidisciplinary": 7/127.*

---

*AUTHORS (in order of authorship): S.H. Choi, C. Risko, M.C. Ruiz Delgado, B. Kim, J.L. Brédas and C. Daniel Frisbie.*

*TITLE: Transition from Tunneling to Hopping Transport in Long, Conjugated Oligo-imine Wires Connected to Metals.*

*JOURNAL/BOOK TITLE: J. Am. Chem. Soc. 132, 4358-4368 (2010) KEY: A*

*DATE OF PUBLICATION (\*): 2010*

*MOST OUTSTANDING ASPECTS (\*\*): Journal impact index (JCR 2008): 8.091; journal position on list of "Chemistry, Multidisciplinary": 7/127.*

---

*AUTHORS (in order of authorship): Roel S. Sánchez-Carrera; M. Carmen Ruiz Delgado\*; Cristina Capel Ferrón; Reyes Malavé Osuna; Víctor Hernández; Juan T. López Navarrete; Alán Aspuru-Guzik*

*TITLE: Optical absorption and emission properties of end-capped oligothienoacenes: A joint theoretical and experimental study*

*JOURNAL/BOOK TITLE: Organic Electronics 11, 1701-1712 (2010) KEY: A*

*DATE OF PUBLICATION (\*): 2010*

MOST OUTSTANDING ASPECTS (\*\*): *Journal impact index (JCR 2008): 8.091; journal position on list of "Chemistry, Multidisciplinary": 7/127.*

---

*AUTHORS (in order of authorship): N. Martinelli; Y. Olivier; L. Muccioli; A. Minoia; P. Brocorens; M.C. Ruiz Delgado; C. Zannoni; D. Beljonne; R. Lazzaroni; J.-L. Brédas; J. Cornil*

*TITLE: Charge Transport in Organic Semiconductors: A Multiscale Modelling*

*JOURNAL/BOOK TITLE: "Functional Supramolecular architectures for organic electronics and nanotechnology". Ed. Wiley-VCH* KEY: CB

*DATE OF PUBLICATION (\*): 2010*

*MOST OUTSTANDING ASPECTS (\*\*): This book supplies an introduction and a review of recent progress in the design, synthesis, development and characterization of functional materials. Our book chapter focuses on the theoretical aspects of the optical and transport properties of conjugated materials for which their supra-molecular arrangement has a particular significance.*

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*AUTHORS (in order of authorship): R. Juárez; M. Moreno Oliva; M. Ramos; J. L. Segura; C. Alemán; F. Rodríguez-Ropero; D. Curcó; F. Montilla; V. Coropceanu; J.L. Brédas; Y. Qi; A. Kahn; M. C. Ruiz Delgado; J. Casado; J. T. López Navarrete*

*TITLE: Hexaazatriphenylene (HAT) versus tri-HAT: The Bigger the Better?*

*JOURNAL/BOOK TITLE: Chemistry A European Journal 17, 10312 – 10322 (2011) KEY: A*

*DATE OF PUBLICATION (\*): 2011*

*MOST OUTSTANDING ASPECTS (\*\*): Journal impact index (JCR 2008): 5.484; journal position on list of "Chemistry, Multidisciplinary": 12/127.*

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*AUTHORS (in order of authorship): Ted M. Pappenfus; Deborah K. Schneiderman; Juan Casado; Juan T. López Navarrete; M. Carmen Ruiz Delgado; Gianni Zotti; Barbara Vercelli; Matthew D. Lovander; Lindsay M. Hinkle; Jon N. Bohnsack; Kent R. Mann*

*TITLE: Oligothiophene Tetracyanobutadienes: Alternative Donor-Acceptor Architectures for Molecular and Polymeric Materials*

*JOURNAL/BOOK TITLE: Chemistry of Materials 23, 823-831 (2011) KEY: A*

*DATE OF PUBLICATION (\*): 2011*

*MOST OUTSTANDING ASPECTS (\*\*): Journal impact index (JCR 2008): 5.046; journal position on list of "Materials Science, Multidisciplinary": 14/192.*

---

*AUTHORS (in order of authorship): C. Capel Ferrón; M. C. Ruiz Delgado\*; V. Hernández; J. T. López Navarrete; B. Vercelli; G. Zotti; M. Capdevila Cortada; J. J. Novoa; W. Niu; M. He; F. Hartl; J. T. López Navarrete*

*TITLE: Substituent and counterion effects on the formation of  $\pi$ -dimer dications of end-capped heptathienoacenes*

*JOURNAL/BOOK TITLE: Chemical Communications, 2011, 47, 12622–12624 (2011) KEY: A*

*DATE OF PUBLICATION (\*): 2011*

MOST OUTSTANDING ASPECTS (\*\*): *Journal impact index (JCR 2010): 5.787; journal position on list of "Materials Science, Multidisciplinary": 17/147*

---

*AUTHORS (in order of authorship):* R. Ponce Ortiz, M. Carmen Ruiz Delgado, J. Casado, V. Hernández and J.T. López Navarrete

*TITLE: The VIII - Spanish National School on Molecular Materials (VIII-ENMM): A Tool to Complement the Scientific Training of Ph.D. and Master Students in Materials Science*

*JOURNAL/BOOK TITLE:* Journal of Materials Education, 33, 13-26 (2011) *KEY:* A

*DATE OF PUBLICATION (\*):* 2011

*MOST OUTSTANDING ASPECTS (\*\*):* *Education, Scientific Disciplines; Materials Science, Multidisciplinary. Subject Category: Education & Educational Research; Materials Science*

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*AUTHORS (in order of authorship):* Sean J. Evenson, Ted M. Pappenfus, M. Carmen Ruiz Delgado, Karla R. Radke-Wohlers, J. T. López Navarrete, and Seth C. Rasmussen

*TITLE: Molecular Tuning in Highly Fluorescent Dithieno[3,2-b:2',3'-d]pyrrole-based Oligomers: Effects of N-Functionalization and Terminal Aryl Unit*

*JOURNAL/BOOK TITLE:* Phys. Chem. Chem. Phys., 14, 6101–6111 (2012) *KEY:* A

*DATE OF PUBLICATION (\*):* 2012

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*AUTHORS (in order of authorship):* Sandra Rodríguez González; M. Carmen Ruiz Delgado; Rubén Caballero; Pilar De la Cruz; Fernando Langa; Juan T. López Navarrete; Juan Casado

*TITLE: Delocalization-to-Localization Charge Transition in Diferrocenyl-Oligothiénylene-Vinylene Molecular Wires as a Function of the Size by Raman Spectroscopy*

*JOURNAL/BOOK TITLE:* Journal of American Chemical Society, 134, 5675–5681 (2012) *KEY:* A

*DATE OF PUBLICATION (\*):* 2012

*MOST OUTSTANDING ASPECTS (\*\*):* *Education, Scientific Disciplines; Materials Science, Multidisciplinary. Subject Category: Education & Educational Research; Materials Science*

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*AUTHORS (in order of authorship):* Cristina Capel Ferrón; M. Carmen Ruiz Delgado; Ori Gidron; Sagar Sharma; Dennis Sheberla; Yana Sheynin; Michael Bendikov; Juan T. López Navarrete; Víctor Hernández

*TITLE:  $\alpha$ -Oligofurans show a sizeable extent of  $\pi$ -conjugation as probed by Raman spectroscopy*

*JOURNAL/BOOK TITLE:* Chemical Communications, Chem. Commun. 48, 6732–6734 (2012) *KEY:* A

*DATE OF PUBLICATION (\*):* 2012

*MOST OUTSTANDING ASPECTS (\*\*):* *Journal impact index (JCR 2010): 5.787; journal position on list of "Materials Science, Multidisciplinary": 17/147*

---

*AUTHORS (in order of authorship):* T. M. Pappenfus, K. B. Schliep, A. Dissanayake, T. Ludden, J. Casado, M. Carmen Ruiz Delgado, B. Nieto Ortega, J. Teodomiro López Navarrete

*TITLE: Organic Materials in the Undergraduate Laboratory: Microscale Synthesis and Investigation of a Donor-Acceptor Molecule*

*JOURNAL/BOOK TITLE: Journal of Chemical Education 89, 1461–1465 (2012) KEY: A*

*DATE OF PUBLICATION (\*): 2012*

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*AUTHORS (in order of authorship):* Rafael C. González Cano; Helena Herrera; José L. Segura; Juan T. López Navarrete; M. Carmen Ruiz Delgado; Juan Casado

*TITLE: Conformational Control of the Electronic Properties of an  $\alpha$ - $\beta$  Terthiophene: Lessons from a Precursor Towards Dendritic Hyperbranched Oligo- and Poly-Thiophenes*

*JOURNAL/BOOK TITLE: ChemPhysChem 13, 3893-3900 (2012) KEY: A*

*DATE OF PUBLICATION (\*): 2012*

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*AUTHORS (in order of authorship):* F. S. U. Fischer; K. Tremel; A. K. Saur; S. Link; N. Kayunkid; M. Brinkmann; D. Herrero-Carvajal; J. T. López Navarrete; M. C. Ruiz Delgado; S. Ludwigs

*TITLE: Influence of Processing Solvents on Optical Properties and Morphology of a Semicrystalline Low Bandgap Polymer in the Neutral and Charged States*

*JOURNAL/BOOK TITLE: Macromolecules 46, 4924-4931 (2013). KEY: A*

*DATE OF PUBLICATION (\*): 2013*

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*AUTHORS (in order of authorship):* Rafael C. González-Cano; G. Saini; J. Jacob; Juan T. López Navarrete; Juan Casado; **M. Carmen Ruiz Delgado\***

*TITLE: Interplay of  $\alpha,\alpha$  versus  $\alpha,\beta$ -conjugation into the Excited States and Charged Defects of Branched Oligothiophenes as Models for Dendrimeric Materials*

*JOURNAL/BOOK TITLE: Chemistry A European Journal 19, 17165 (2013). KEY: A*

*DATE OF PUBLICATION (\*):*

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*AUTHORS (in order of authorship):* Nur S. Rizalman; Cristina Capel Ferron; Weijun Niu; Arthur L. Wallace; Mingqian He; Russell Balster; John Lampkin; Víctor Hernandez; Juan T López Navarrete; **M. Carmen Ruiz Delgado\***; Frantisek Hartl

*TITLE: Radical cations of end-capped tetrathienoacenes and their  $\pi$ -dimerization controlled by the nature of alpha-substituents and counterion concentration.*

*JOURNAL/BOOK TITLE: RSC Advances 3, 25644 (2013). KEY: A*

*DATE OF PUBLICATION (\*):*

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*AUTHORS (in order of authorship):* Steffen Link; Martin Scheuble; Miriam Goll; Erna Muks; Adrian Ruff; Anke Hoffmann; Thomas V. Richter; Juan T. Lopez Navarrete; M. Carmen Ruiz Delgado; Sabine Ludwigs



*TITLE: Electropolymerized Three-Dimensional Randomly Branched EDOT-Containing Copolymers*

*JOURNAL/BOOK TITLE: Langmuir 29, 15463 (2013). KEY: A*

*DATE OF PUBLICATION (\*):*

*langmuir*

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*AUTHORS (in order of authorship):* José Luis Zafra; Rafael C. Gonzalez Cano; M. Carmen Ruiz Delgado; Zhe Sun; Yuan Li; Juan T. Lopez Navarrete; Jishan Wu; J. Casado.

*TITLE: Zethrene biradicals: How pro-aromaticity is expressed in the ground electronic state and in the lowest energy singlet, triplet, and ionic states*

*JOURNAL/BOOK TITLE: Journal of Chemical Physics 140, 054706 (2014). KEY: A*

*DATE OF PUBLICATION (\*):*

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*AUTHORS (in order of authorship):* Constanza Ruiz; Eva M. García-Frutos; Demetrio A. da Silva Filho; Juan T. López Navarrete; **M. Carmen Ruiz Delgado\***; Berta Gómez-Lor

*TITLE: Symmetry Lowering in Triindoles: Impact on the Electronic and Photophysical Properties*

*JOURNAL/BOOK TITLE: J. Phys. Chem. C, 118, 5470 (2014) KEY: A*

*DATE OF PUBLICATION (\*):*

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*AUTHORS (in order of authorship):* Daniel Herrero-Carvajal; Alejandro de la Peña; Rafael C. González Cano; Carlos Seoane; Juan T. López Navarrete; José L. Segura; Juan Casado; **M. Carmen Ruiz Delgado\***

*TITLE: EDOT-Based Copolymers with Pendant Anthraquinone Units: Analysis of Their Optoelectronic Properties within the Double-Cable Context*

*JOURNAL/BOOK TITLE: J. Phys. Chem. C, 118, 9899 (2014) KEY: A*

*DATE OF PUBLICATION (\*):*

---

*AUTHORS (in order of authorship):* C. Capel Ferrón; Y. Sheynin; M. Li; A. Patra; M. Bendikov; Juan T. López Navarrete; V. Hernández; **M. Carmen Ruiz Delgado\***

*TITLE: Raman Spectroscopic Characterization of Polyselenophenes and Poly(3,4-ethylenedioxyselenophene)s*

*JOURNAL/BOOK TITLE: Israel Journal of Chemistry, 54, 759 (2014)*

*DATE OF PUBLICATION (\*):*

---

*AUTHORS (in order of authorship):* Cristina Capel Ferrón; Marçal Capdevila-Cortada; Russell Balster; František Hartl; Weijun Niu; Mingqian He; Juan J. Novoa; Juan T. López Navarrete; Víctor Hernández; **M. Carmen Ruiz Delgado\***

*TITLE: Multistep pi-Dimerization of Tetrakis(n-decyl)-heptathienoacene Radical Cations: A Combined Experimental and Theoretical Study*

*JOURNAL/BOOK TITLE: Chemistry A European Journal, 20, 10351 (2014)*

) KEY: A

DATE OF PUBLICATION (\*):

---

*AUTHORS (in order of authorship): Jonas Sjöqvist; Rafael C. González-Cano; J.T. López Navarrete; J. Casado; M.C. Ruiz Delgado; M. Linares; P. Norman.*

*TITLE: A combined MD/QM and experimental exploration of conformational richness in branched oligothiophenes..*

*JOURNAL/BOOK TITLE: Physical Chemistry Chemical Physics. 16, 24841 (2014)*

KEY: A

DATE OF PUBLICATION (\*):

---

*AUTHORS (in order of authorship): M. Scheuble; T.V. Richter; M. Goll; S. Link; Juan T. López Navarrete; A. Ruff; M.Carmen Ruiz Delgado; S. Ludwigs.*

*TITLE: Branched polythiophenes by Ni-catalyzed Kumada coupling.*

*JOURNAL/BOOK TITLE: Polymer Chemistry. 5, 6824 – 6833 (2014)*

KEY: A

DATE OF PUBLICATION (\*):

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*AUTHORS (in order of authorship): Miriam Goll, Adrian Ruff, Erna Muks, Felix Goerigk, Beatrice Omiecienski, Ines Ruff,, Rafael C. González-Cano, Juan T. Lopez Navarrete, M. Carmen Ruiz Delgado and Sabine Ludwigs*

*TITLE: Functionalized branched EDOT-terthiophene copolymer films by electropolymerization and post-polymerization "click"-reactions*

*JOURNAL/BOOK TITLE: BEILSTEIN JOURNAL OF ORGANIC CHEMISTRY, 11, 335 (2015)*

) KEY: A

DATE OF PUBLICATION (\*):

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*AUTHORS (in order of authorship): Constanza Ruiz, Juan T. López Navarrete, M. Carmen Ruiz Delgado\*, and Berta Gómez-Lor*

*TITLE: Triindole-Bridge-Triindole Dimers as Models for Two Dimensional Microporous Polymers*

*JOURNAL/BOOK TITLE: Organic Letters 17, 2258–2261 (2015)*

KEY: A

DATE OF PUBLICATION (\*):

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*AUTHORS (in order of authorship): M. Scheuble, Y. M. Gross, D. Trefz, M. Brinkmann, J. T. López Navarrete, M. C. Ruiz Delgado, S. Ludwigs*

*TITLE: Polythiophenes with Thiophene Side Chain Extensions: Convergent Syntheses and Investigation of Mesoscopic Order*

JOURNAL/BOOK TITLE: *Macromolecules*, 48, 7049–7059 (2015)

KEY: A

DATE OF PUBLICATION (\*):

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AUTHORS (in order of authorship): *Miriam Peña-Alvarez, Lili Qiu, Mercedes Taravillo, Valentí G. Baonza, M. Carmen Ruiz Delgado, Shigeru Yamago, Ramesh Jasti, Juan T. López Navarrete, Juan Casado, Miklos Kertesz*

TITLE: *From linear to cyclic oligoparaphenylenes: electronic and molecular changes traced in the vibrational Raman spectra and reformulation of the bond length alternation pattern*

JOURNAL/BOOK TITLE: *Phys. Chem. Chem. Phys.* 18, 11683-11692 (2016)

KEY: A

DATE OF PUBLICATION (\*):

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AUTHORS (in order of authorship): *M. K. Poduval, Iratxe Arrechea-Marcos, M. Carmen Ruiz Delgado, Taiho Park, J. Teodomiro Lopez Navarrete, Rocio Ponce Ortiz, Tae-Hyun Kim*

TITLE: *Stereoisomers of an azine-linked donor-acceptor conjugated polymer: the impact of molecular conformation on electrical performance*

JOURNAL/BOOK TITLE: *RSC Advances* 6, 44272-44278 (2016)

KEY: A

DATE OF PUBLICATION (\*):

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AUTHORS (in order of authorship): *Miriam Peña Alvarez, M. Carmen Ruiz Delgado, Mercedes Taravillo, Valentín G. Baonza, Juan T. López Navarrete, Paul Evans, Ramesh Jasti, Shigeru Yamago, Miklos Kertesz, Juan Casado*

TITLE: *The Raman fingerprint of cyclic conjugation: the case of the stabilization of cations and dications in cycloparaphenylenes*

JOURNAL/BOOK TITLE: *Chem. Sci.* 7, 3494-3499 (2016)

KEY: A

DATE OF PUBLICATION (\*):

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AUTHORS (in order of authorship): *Constanza Ruiz, Ángeles Monge, Enrique Gutiérrez-Puebla, Ibon Alkorta, José Elguero, Juan T. López Navarrete, M. Carmen Ruiz Delgado\*, Berta Gómez-Lor*

TITLE: *Saddle-Shaped Cyclic Indole Tetramers: 3D Electroactive Molecules*

JOURNAL/BOOK TITLE: *Chemistry A European Journal*, 22, 10651 – 10660 (2016)

KEY: A

DATE OF PUBLICATION (\*):

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*AUTHORS (in order of authorship): Alejandro de la Peña, Iratxe Arrechea-Marcos, María J. Mancheño, M. Carmen Ruiz Delgado, J. Teodomiro López Navarrete, José L. Segura, Rocío Ponce Ortiz*

*TITLE: Tuning of the Electronic Levels of Oligothiophene–Naphthalimide Assemblies by Chemical Modification*

*JOURNAL/BOOK TITLE: Chemistry A European Journal, 22, 13643 – 13652 (2016)*

*KEY: A*

*DATE OF PUBLICATION (\*):*

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*AUTHORS (in order of authorship): Constanza Ruiz, Upendra Kumar Pandey, Roberto Termine, Eva María García-Frutos, Guzmán López-Espejo, Rocío Ponce Ortiz, Wei Huang, Tobin J. Marks, Antonio Facchetti, M. Carmen Ruiz Delgado, Attilio Golemme, and Berta Gómez-Lor*

*TITLE: Mobility vs Alignment of a Semiconducting  $\pi$ -Extended Discotic Liquid-crystalline Triindole*

*JOURNAL/BOOK TITLE: ACS Appl. Mater. Interfaces, Just Accepted*

*DOI: 10.1021/acsami.6b06241*

*KEY: A*

*DATE OF PUBLICATION (\*):*

### **MOST OUTSTANDING PUBLICATIONS**

**(Select the five publications that you consider to be the most outstanding ones. Include for each of them a brief summary with its most notable objectives and results)**

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*AUTHORS (in order of authorship): M.C. Ruiz Delgado, E.G. Kim, D.A. da Silva Filho, J.L. Brédas.*

*TITLE: Tuning the Charge-Transport Parameters of Perylene Diimide Single Crystals via End and/or Core Functionalization: A Density Functional Theory Investigation.*

*JOURNAL/BOOK TITLE: J. Am. Chem. Soc. 132, 3375-3387 (2010)      KEY: A*

*DATE OF PUBLICATION (\*): 2010*

*MOST OUTSTANDING ASPECTS (\*\*): Research work performed during my postdoctoral stay at the Georgia Institute of Technology. Manuscript published in one of the journals with the highest impact index in the Chemistry field. Journal impact index (JCR 2008): 8.091; journal position on list of "Chemistry, Multidisciplinary": 7/127. This work presents a very exhaustive theoretical study performed over 37 perylene-based (PTCDI) crystal structures, all of the PTCDI chemical structures found in the Cambridge Database. We analyze the impact of functionalization (core- and end-substitution) on the charge-transport parameters of these materials. While the molecular electronic properties are only slightly influenced by the nature and positions of the substituents, the solid-state packing and resulting charge-transport properties are strongly affected. Wide hole- and electron-transport bands and small effective masses are obtained with the insertion of appropriate substituents on the nitrogen atoms, in particular halogenated aromatic groups. These results allowed us to identify a number of PTCDI crystals that are still to be examined experimentally and are predicted to display outstanding hole- and/or electron-transport characteristics.*

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AUTHORS (in order of authorship): M.C. Ruiz Delgado, K. R. Pigg, D.A. da Silva Filho, N. E. Gruhn, Y. Sakamoto, T. Suzuki, R. Malave, J. Casado, V. Hernández, J.T. López Navarrete, N. G. Martinelli, J. Cornil, R.S. Sánchez-Carrera, V. Coropceanu, J.L. Brédas.

TITLE: *Impact of Perfluorination on the Charge-Transport Parameters of Oligoacene Crystals.*

JOURNAL/BOOK TITLE: J. Am. Chem. Soc. 131, 1502-1512 (2009)

KEY: A

DATE OF PUBLICATION (\*): 2009

MOST OUTSTANDING ASPECTS (\*\*): *Research work performed during my postdoctoral stay at the Georgia Institute of Technology. Manuscript published in one of the journals with the highest impact index in the Chemistry field. Journal impact index (JCR 2008): 8.091; journal position on list of "Chemistry, Multidisciplinary": 7/127. In this manuscript, we investigate the role of perfluorination on the charge-transport properties of oligoacene crystals by using a joint theoretical and experimental approach (gas-phase UPS and DFT calculations). These results reveals that both electronic and electron-phonon interactions are very sensitive to the insertion of the fluorine atoms. In the perfluorinated crystals, we find significant electronic couplings and very small effective masses for both holes and electrons along the  $\pi$ -stack direction. Interestingly, our calculations reveal larger electronic couplings for holes than for electrons and similar electron-phonon coupling for holes and electrons in the perfluorinated crystals, which suggest that one might expect these materials to act as ambipolar charge transporters under proper operating conditions.*

---

AUTHORS (in order of authorship): S. Salman, M.C. Ruiz Delgado, V. Coropceanu, J.L. Brédas.

TITLE: *Electronic Structure and Charge-Transport Parameters of Functionalized Tetracene Crystals: Impact of Partial Fluorination and Alkyl or Alkoxy Derivatization.*

JOURNAL/BOOK TITLE: Chemistry of Materials 21, 3593-3601 (2009)

KEY: A

DATE OF PUBLICATION (\*): 2009

MOST OUTSTANDING ASPECTS (\*\*): *Research work performed during my postdoctoral stay at the Georgia Institute of Technology as a main author. My scientific contribution to this manuscript was very important: I directed the research of the PhD student Seyhan Salman as a principal investigator of this work. Manuscript published in one of the journals with the highest impact index in the Materials Science field. Journal impact index (JCR 2008): 5.046; journal position on list of "Materials Science, Multidisciplinary": 14/192. My contribution to this manuscript was very significant since I conducted and directed the research. The charge transport parameters of  $\pi$ -stacking tetracene crystals are investigated here by using DFT theory calculations. Our goal is to gain a better understanding of the role of partial fluorination, which trigger the formation of alternating face-to-face stacks, and alkyl/alkoxy substitution. The incorporation of both donor and acceptor substituents to the tetracene is found to increase the reorganization energy. The largest electron mobility is predicted for the material where alkyl substitution leads to a simple  $\pi$ -stacking motif. We have been able to identify promising candidates to be used in OFETs.*

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AUTHORS (in order of authorship): M. Carmen Ruiz Delgado, J. Casado, V. Hernández, J.T. López Navarrete, J. Orduna, B. Villacampa, R. Alicante, J.-M. Raimundo, P. Blanchard, J. Roncali.

TITLE: *Electronic, Optical, and Vibrational Properties of Bridged Dithienylethylene-Based NLO Chromophores.*

JOURNAL/BOOK TITLE: J. Phys. Chem. C, 112, 3109-3120 (2008).

KEY: A

DATE OF PUBLICATION (\*): 2008

MOST OUTSTANDING ASPECTS (\*\*): *Manuscript published in one of the journals with the highest impact index in the Materials Science field during my postdoctoral stay at the Institute of Materials Science of Aragón. Journal impact index (JCR 2008): 3.396; journal position on list of "Materials Science, Multidisciplinary": 26/192. In this multidisciplinary work, we evaluate the second-order NLO properties of a series of organic push-pull molecules by using Density Functional Theory calculations, vibrational spectroscopy and EFISH measurements. Chromophores built around a covalently rigidified DTE spacer and bearing a strong acceptor display the highest NLO response. The spectroscopic/structure relationships are in good agreement with the NLO measurements interpreted upon assumption of a higher polarization of the ground electronic state for systems with covalently bridged spacers and strong electron acceptors.*

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*AUTHORS (in order of authorship): M. C. Ruiz Delgado, J. Casado, V. Hernández, J. T. López Navarrete, G. Fuhrmann and P. Bäuerle.*

*TITLE: Combined Raman and Computational Study of a Novel Series of Macrocyclic  $\pi$ -Conjugated Diacetylene-Bridged  $\alpha$ -linked Oligothiophenes.*

*JOURNAL/BOOK TITLE: J. Phys. Chem. B 108, 3158-3167 (2004). KEY: A*

*DATE OF PUBLICATION (\*): 2004*

*MOST OUTSTANDING ASPECTS (\*\*): Manuscript published during the PhD period in a high impact journal in the Physical Chemistry field. Journal impact index (JCR 2008): 4.189; journal position on list of "Chemistry,Physical": 22/113; cites received: 22 (isi web of knowledge). The scientific quality of this work is supported by the achievement of the Young Scientist Award by the "Fundación General de la Universidad de Málaga".*

In this work, we present a study of macrocyclic molecular materials which combine the advantages of a structurally well-defined oligomer but lacking of any perturbing end-effects. By combining theoretical calculations and vibrational spectroscopy, we analyze the efficiency of the  $\pi$ -conjugation in these macrocyclic oligothiophenes. The effective  $\pi$ -conjugation is found to be almost independent of the molecular conformation of the macrocycle. The evolution of the Raman spectra with the temperature reveals that these molecular materials are thermally stable at least up to +150 °C which gives support to their potential application in technological devices.

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## STAYS IN INTERNATIONALLY RECOGNIZED CENTRES

KEY: D=Ph.D student, P=postdoctoral. G= guest, S=staff, O=others (specify)

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*CENTRE: Department of Physical Chemistry, University of Valencia (SPAIN)*  
*PLACE: Valencia COUNTRY: Spain YEAR: 2003 LENGHT: 12 weeks*  
*TOPIC: Vibrational spectroscopy study of conjugated oligomers by means of quantum chemical DFT calculations*  
*KEY: D*  
Supervisor: Prof. Dr. Enrique Ortí Guillén

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*CENTRE: Department of Organic Chemistry, Institute of Materials Science of Aragón*  
*PLACE: Zaragoza COUNTRY: Spain YEAR: 2004 LENGHT: 16 weeks*  
*TOPIC: Evaluation of the Second Order Non Linear Optical Properties in Push-Pull Materials by using Quantum chemical DFT calculations*  
*KEY: D*  
Supervisor: Prof. Dr. Jesús Orduna Catalán

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*CENTRE: School of Chemistry and Biochemistry. Georgia Institute of Technology*  
*PLACE: Atlanta COUNTRY: USA YEAR: 2005 LENGHT: 16 weeks*  
*TOPIC: Charge-transport properties in Organic Semiconductors*  
*KEY: D*  
Supervisor: Prof. Dr. Jean-Luc Brédas

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*CENTRE: Department of Organic Chemistry, Institute of Materials Science of Aragón*  
*PLACE: Zaragoza COUNTRY: Spain YEAR: 2007 LENGHT: From 15/01/2007 to 23/03/2007*  
*TOPIC: Theoretical Study of the Second Order Non Linear Optical Properties in Octupolar Molecules*  
*KEY: P*  
Supervisor: Prof. Dr. Jesús Orduna Catalán

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*CENTRE: School of Chemistry and Biochemistry. Georgia Institute of Technology*  
*PLACE: Atlanta COUNTRY: USA YEAR: 2007-2010 LENGHT: From 01/04/2007 to 31/03/2010*  
*TOPIC: Study of the intermolecular interactions impact on the optical, electrical and charge-transport properties in Conjugated Materials*  
*KEY: P*  
Supervisor: Prof. Dr. Jean-Luc Brédas

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*CENTRE: University of Stuttgart*  
*PLACE: Stuttgart COUNTRY: Alemania YEAR: 2012 LENGHT: From 18/04/2012 to 20/04/2012*  
*TOPIC: Investigation of the electronic and charge-transport properties of organic semiconductors by using DFT calculations*  
*KEY: P*  
Supervisor: Prof. Dr. Sabine Ludwigs

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*CENTRE: University of Cergy-Pointoise*  
*PLACE: Cergy COUNTRY: France YEAR: 2014 LENGHT: From 10/03/2014 to 14/03/2014*  
*TOPIC: Investigation of the optical and electronic properties of organic semiconductors: a combined experimental and theoretical approach*  
*KEY: P*  
Supervisor: Prof. Dr. Gjergji Sini

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## PRESENTATIONS IN CONGRESSES

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*AUTHORS: C. Moreno Castro, M.C. Ruiz Delgado, V. Hernández, S. Hotta, J. Casado and J. T. López Navarrete.*

*TITLE: Raman Spectra of a Novel Family of Thiophene/Phenylene co-oligomers in Neutral and Doped States.*

*TYPE OF PRESENTATION: Publicación.*

*CONGRESS: XVIII International Conference on Raman Spectroscopy (ICORS 2002).*

*MEETING PLACE: Budapest, Hungary*

*YEAR: 25-30 August 2002.*

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*AUTHORS: J. Casado, M.C. Ruiz Delgado, V. Hernández, J. T. López Navarrete, J-M Raimundo, P. Blanchard and J. Roncali.*

*TITLE: Vibrational Study of Push-Pull Chromophores for Second Order Nonlinear Optics Derived From Rigidified Thiophene-Based- $\pi$ -Conjugating Spacer .*

*TYPE OF PRESENTATION: Comunicación Oral OB1.*

*CONGRESS: XXVI European Congress on Molecular Spectroscopy*

*MEETING PLACE: Villeneuve d'Ascq, France.*

*YEAR: 1-6 September 2002.*

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*AUTHORS: J. Casado, M.C. Ruiz Delgado, V. Hernández, J. T. López Navarrete, B. Millán, P. M. Viruela and E. Ortí.*

*TITLE: UV-VIS, IR, Raman and Theoretical Characterization of a Novel Type of Quinoid Oligothiophene Molecular Material.*

*TYPE OF PRESENTATION: Comunicación Poster P13.3.*

*CONGRESS: XXVI European Congress on Molecular Spectroscopy*

*MEETING PLACE: Villeneuve d'Ascq, France.*

*YEAR: 1-6 September 2002.*

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*AUTHORS: M.C. Ruiz Delgado, V. Hernández, J. Casado, J. T. López Navarrete, J.M. Raimundo, P. Blanchard and J. Roncali.*

*TITLE: Infrared and Raman Spectroscopic Study, in Solid State and Solution , of Push-Pull Chromophores for Second-Order Nonlinear Optics Derived from Rigidified Thiophene-Based  $\pi$ -Conjugating Spacers.*

*TYPE OF PRESENTATION: Comunicación Poster 5541-0123.*

*CONGRESS: 5<sup>th</sup> International Symposium on Functional  $\pi$ -Electron Systems.*

*MEETING PLACE: Ulm/Neu-Ulm Germany.*

*YEAR: May 30-June 4, 2002.*

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*AUTHORS: C. Moreno Castro, M.C. Ruiz Delgado, V. Hernández, Y. Shirota and J. T. López Navarrete.*

*TITLE: Vibrational Spectroscopy Features of a Novel Family of Amorphous Molecular Materials Containing an oligothiophene Moiety as Colour-Tunable Emitting materials.*

*TYPE OF PRESENTATION: Comunicación Poster 5541-0150.*

*CONGRESS: 5<sup>th</sup> International Symposium on Functional  $\pi$ -Electron Systems.*

*MEETING PLACE: Ulm/Neu-Ulm Germany.*

*YEAR: May 30-June 4, 2002.*

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AUTHORS: M.C. Ruiz Delgado, V. Hernández, J. Casado, J. T. López Navarrete, G. Fuhrmann, A. Kaiser and P. Bauerle.

TITLE: : Infrared and Raman Study of a Series of Macrocyclic  $\pi$ -Conjugated Diacetylene-Bridged  $\alpha$ -linked Oligothiophenes in Neutral and Doped States.

TYPE OF PRESENTATION: Comunicación Poster 5541-0127.

CONGRESS: 5<sup>th</sup> International Symposium on Functional  $\pi$ -Electron Systems.

MEETING PLACE: Ulm/Neu-Ulm Germany.

YEAR: May 30-June 4, 2002.

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AUTHORS: J. T. López Navarrete, J. Casado, M.C. Ruiz Delgado, V. Hernández, J.M. Raimundo, P. Blanchard and J. Roncali.

TITLE: Caracterización por espectroscopía Infrarroja y Raman, y métodos químico-cuánticos de oligotiofenos sustituidos con grupos dadores y aceptores de electrones con aplicaciones en óptica no-lineal de segundo orden.

TYPE OF PRESENTATION: Comunicación Poster.

CONGRESS: Bienal Centenario de la Real Sociedad Española de Química y Física (RSEQ 2003)

MEETING PLACE: Madrid, España

YEAR: 25-30 July 2003.

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AUTHORS: S. Delgado Ledesma, M.C. Ruiz Delgado, V. Hernández, J. T. López Navarrete, O.-K. Kim, J.-M. Lehn.

TITLE: Espectroscopias UV-VIS-NIR, IR y Raman y cálculos químico-cuánticos DFT y TDDFT sobre cromóforos orgánicos para óptica no lineal de segundo orden, conteniendo un ditienotiofeno  $\pi$ -conjugado central.

TYPE OF PRESENTATION: Comunicación Oral A2.

CONGRESS: VI Escuela Nacional de Materiales Moleculares 2003

MEETING PLACE: L'Azohia, Cartagena, España.

YEAR: 21-29 June 2003.

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AUTHORS: M.C. Ruiz Delgado, V. Hernández, J. Casado, J.T. López Navarrete, J.M. Raimundo, P. Blanchard, J. Roncali.

TITLE: Estudio espectroscópico (UV-VIS-NIR, IR y Raman) y computacional (DFT y TDDFT) de cromóforos orgánicos para óptica no-lineal de segundo orden, con espaciadores  $\pi$ -conjugados centrales bitiofénicos rigidificados.

TYPE OF PRESENTATION: Comunicación Oral A3.

CONGRESS: VI Escuela Nacional de Materiales Moleculares 2003

MEETING PLACE: L'Azohia, Cartagena, España.

YEAR: 21-29 June 2003.

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AUTHORS: M.C. Ruiz Delgado, V. Hernández, J. Casado, J.T. López Navarrete, J.M. Raimundo, P. Blanchard, J. Roncali.

TITLE: Caracterización químico-cuántica (DFT y TDDFT) y espectroscópica de cromóforos dador aceptor para óptica no-lineal de segundo orden: moléculas con espaciadores  $\pi$ -conjugados oligotiofénicos rigidificados.

TYPE OF PRESENTATION: Comunicación Poster P-50.

CONGRESS: 29<sup>ème</sup> Congrès International des Chimistes Théoriciens d'Expression Latine

MEETING PLACE: Marrakech, Marroco.

YEAR: 07-12 September 2003

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*AUTHORS: M.C. Ruiz Delgado, V. Hernández, J. Casado, Rocio Ponce, J.T. López Navarrete, J.M. Raimundo, P. Blanchard, J. Roncali.*  
*TITLE: Quantum-Chemical (DFT and TDDFT) and Vibrational Study of Push-Pull Chromophores for Second Order-Nonlinear Optics Devices.*  
*TYPE OF PRESENTATION: Comunicación Oral.*  
*CONGRESS: 4th Workshop of conjugated oligomers and polymers from synthesis to electronic function.*  
*MEETING PLACE: Ulm, Germany.*  
*YEAR: on 2-5 November 2003.*

---

*AUTHORS: M.C. Ruiz Delgado, V. Hernández, J. Casado, J.T. López Navarrete, Shoji Tanaka and Yoshiro Yamashita.*  
*TITLE: Vibrational Spectroscopy and theoretical study of narrow-bandgap heterocyclic cooligomers containing alternating aromatic-donor and o-quinoid-acceptor units.*  
*TYPE OF PRESENTATION: Comunicación Oral.*  
*CONGRESS: 4th Workshop of conjugated oligomers and polymers from synthesis to electronic function.*  
*MEETING PLACE: Ulm, Germany.*  
*YEAR: on 2-5 November 2003.*

---

*AUTHORS: R. Ponce Ortiz, M. C. Ruiz Delgado, J. Casado, V. Hernández, O-K. Kim, J. T. López Navarrete.*  
*TITLE: In situ spectroelectrochemical and quantum chemical DFT study of some D- $\pi$ -D chromophores bearing dithienothiopene, DTT, as  $\pi$ -center, and showing unusual amphoteric redox properties.*  
*TYPE OF PRESENTATION: Comunicación Oral ME-D1.*  
*CONGRESS: Internacional Conference on Synthetic Metals ICSM 2004*  
*MEETING PLACE: Wollongong, Australia.*  
*YEAR: 28 June-2 July 2004.*

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*AUTHORS: M. C. Ruiz Delgado, R. Ponce Ortiz, J. Casado, P. Blanchard, J. Roncali, V. Hernández, J. T. López Navarrete.*  
*TITLE: Synthesis, cyclic voltammetry, UV-VIS-NIR and FT-Raman spectroscopies and DFT theoretical study of narrow-bandgap  $\pi$ -conjugated mixed heterocyclic trimers containing EDOT donor and thienopyrazine acceptor units.*  
*TYPE OF PRESENTATION: Comunicación tipo póster P66.*  
*CONGRESS: Internacional Conference on Synthetic Metals ICSM 2004*  
*MEETING PLACE: Wollongong, Australia.*  
*YEAR: 28 June-2 July 2004.*

---

*AUTHORS: M. C. Ruiz Delgado, R. Ponce Ortiz, Y. Yamashita, V. Hernández, J. T. López Navarrete.*  
*TITLE: Combined spectroscopic, electrochemical and theoretical study of a biphenylene-TCNQ and a phenylene-TFF analogues containing fused 1,2,5,-thiadiazole units.*  
*TYPE OF PRESENTATION: Comunicación tipo póster P152.*  
*CONGRESS: Internacional Conference on Synthetic Metals ICSM 2004*  
*MEETING PLACE: Wollongong, Australia.*  
*YEAR: 28 June-2 July 2004.*

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*AUTHORS: J. Casado, R. Ponce Ortiz, M.C. Ruiz Delgado, V. Hernández, J.T. López Navarrete, A.Facchetti, T.J. Marks.*  
*TITLE: Vibrational, Spectroelectrochemical and DFT Studies on a family of fluorocarbon-substituted oligothiophenes showing n-type conduction in Thin Film Transistors.*  
*TYPE OF PRESENTATION: Comunicación tipo póster P154.*

CONGRESS: *Internacional Conference on Synthetic Metals ICSM 2004*

MEETING PLACE: *Wollongong, Australia.*

YEAR: *28 June-2 July 2004.*

---

AUTHORS: *V. Cuberos Guzmán, M. C. Ruiz Delgado, R. Ponce Ortiz, V. Hernández, J. Casado, J.T. López Navarrete, R. Azumi, R. T. Oakley.*

TITLE: *Spectroscopic, Electrochemical and Theoretical Study of oligothiophenes end-capped by nitriles in various redox states.*

TYPE OF PRESENTATION: *Comunicación tipo póster P64.*

CONGRESS: *Internacional Conference on Synthetic Metals ICSM 2004*

MEETING PLACE: *Wollongong, Australia.*

YEAR: *28 June-2 July 2004.*

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AUTHORS: *R. Malavé Osuna, M.C. Ruiz Delgado, J. Casado, S. A. Janeckhe, A.J. Bard, V. Hernández, J.T. López Navarrete.*

TITLE: *Spectroelectrochemical and Quantum Chemical DFT Study of a 3,7-[bis[4-phenyl-2-quinoly]]-10-methylphenothiazine donor-acceptor molecule.*

TYPE OF PRESENTATION: *Comunicación tipo póster P65.*

CONGRESS: *Internacional Conference on Synthetic Metals ICSM 2004*

MEETING PLACE: *Wollongong, Australia.*

YEAR: *28 June-2 July 2004.*

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AUTHORS: *M. C. Rey Merchán, M. C. Ruiz Delgado, J. Casado, P. Blanchard, J. Roncali, V. Hernández, J.T. López Navarrete.*

TITLE: *DFT and UV-VIS-NIR, FT-IR, and FT-Raman Spectroscopic Study of push-pull NLO-phoros containing Edot or 3,4-dihexyloxi-thiophene as the electron relay.*

TYPE OF PRESENTATION: *Comunicación tipo póster P153.*

CONGRESS: *Internacional Conference on Synthetic Metals ICSM 2004*

MEETING PLACE: *Wollongong, Australia.*

YEAR: *28 June-2 July 2004.*

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AUTHORS: *J. Casado, M. C. Ruiz Delgado, R. Ponce Ortiz, V. Hernández, J. T. López Navarrete, R. G. Hicks, D. J. T. Myles.*

TITLE: *Spectroscopic and theoretical DFT study of single and double oxidized mesithyl thio-oligothiophenes as model for electrode-single molecule-electrode devices.*

TYPE OF PRESENTATION: *Comunicación tipo póster AP.39.*

CONGRESS: *Sixth International Symposium on Functional  $\pi$ -Electron Systems F $\pi$ 6.*

MEETING PLACE: *Ithaca, Nueva York, USA.*

YEAR: *14-18 June 2004.*

---

AUTHORS: *R. Ponce Ortiz, M.C. Ruiz Delgado, J. Casado, V. Hernández, O-K. Kim, J.T. López Navarrete.*

TITLE: *In situ spectroelectrochemical and DFT studies of some D- $\pi$ -D chromophores bearing dithienothiophene (DTT) as  $\pi$ -center, and showing unusual amphoteric redox properties.*

TYPE OF PRESENTATION: *Comunicación tipo póster AP.38.*

CONGRESS: *Sixth International Symposium on Functional  $\pi$ -Electron Systems F $\pi$ 6.*

MEETING PLACE: *Ithaca, Nueva York, USA.*

YEAR: *14-18 June 2004.*

---

*AUTHORS: V. Cuberos Guzmán, R. Ponce Ortiz, M. C. Ruiz Delgado, R. Azumi, R.T Oakley, J. Casado, V. Hernández and J. T. López Navarrete.*

*TITLE: Combined Spectroscopic, Electrochemical and quantum-chemical study of a series of oligothiophenes end-capped by nitriles in various redox states.*

*TYPE OF PRESENTATION: Comunicación tipo póster AP.41.*

*CONGRESS: Sixth International Symposium on Functional  $\pi$ -Electron Systems F $\pi$ 6.*

*MEETING PLACE: Ithaca, Nueva York, USA.*

*YEAR: 14-18 June 2004.*

---

*AUTHORS: R. Malavé Osuna, R. Ponce Ortiz, M. C. Ruiz Delgado, E. Perez-Inestrosa, J. Casado, V. Hernández, J. T. López Navarrete.*

*TITLE: Synthesis , Spectroscopic, Cyclic Voltammetric and Quantum Chemical DFT Study of a Narrow-Bandgap  $\pi$ -Conjugated Compound Containing Bithiophene Electron-Donor Units Linked to a Central Electron-Acceptor Di-Cyano-Substituted Pyrazine Moiety.*

*TYPE OF PRESENTATION: Comunicación tipo póster AP.42.*

*CONGRESS: Sixth International Symposium on Functional  $\pi$ -Electron Systems F $\pi$ 6.*

*MEETING PLACE: Ithaca, Nueva York, USA.*

*YEAR: 14-18 June 2004.*

---

*AUTHORS: M. C. Ruiz Delgado, R. Ponce Ortiz, V. Hernández, J. T. López Navarrete, S. Tanaka, and Y. Yamashita.*

*TITLE: Vibrational Spectroscopy and DFT Theoretical Study of Narrow-Bandgap Heterocyclic Cooligomers Containing Alternating Aromatic-Donor and o-Quinoid-Acceptor Units.*

*TYPE OF PRESENTATION: Comunicación tipo póster AP.44.*

*CONGRESS: Sixth International Symposium on Functional  $\pi$ -Electron Systems F $\pi$ 6.*

*MEETING PLACE: Ithaca, Nueva York, USA.*

*YEAR: 14-18 June 2004.*

---

*AUTHORS: R. Ponce Ortiz, M.C. Ruiz Delgado, J. Casado, P. Blanchard, J. Roncali, V. Hernandez, J.T. Lopez Navarrete.*

*TITLE: Synthesis , Spectroscopic, Cyclic Voltammetric, in situ Spectroelectrochemical and DFT Theoretical Study of Narrow-Bandgap  $\pi$ -Conjugated Mixed Heterocyclic Trimers Containing EDOT Electron-Donor Units Linked to a Central Electron-Acceptor Thienopyrazine Moiety.*

*TYPE OF PRESENTATION: Comunicación tipo póster AP.43.*

*CONGRESS: Sixth International Symposium on Functional  $\pi$ -Electron Systems F $\pi$ 6.*

*MEETING PLACE: Ithaca, Nueva York, USA.*

*YEAR: 14-18 June 2004.*

---

*AUTHORS: S. Delgado Ledesma, M.C. Ruiz Delgado, V. Hernández, J. Casado, R. Ponce Ortiz, J. T. López Navarrete, O.-K. Kim, J.-M. Lehn.*

*TITLE: Estudio espectroscópico y computacional de cromóforos orgánicos para óptica no-lineal de segundo orden, conteniendo un espaciador  $\pi$ -conjugado ditiotenotiofénico (DTT) central.*

*TYPE OF PRESENTATION: Comunicación tipo póster PM-12.*

*CONGRESS: XIX Reunión Nacional de Espectroscopía.*

*MEETING PLACE: Canarias, España.*

*YEAR: July 2004.*

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*AUTHORS: S. Delgado Ledesma; R. Ponce Ortiz; M.C. Ruiz Delgado; Y. Vida; E. Pérez-Inestrosa, J. Casado; V. Hernández; O-K. Kim; J.-M. Lehn; J.T. López Navarrete.*  
*TITLE: Vibrational and Quantum-Chemical Study of push-pull Chromophores bearing Dithienothiophene as the Electron Relay.*  
*TYPE OF PRESENTATION: Comunicación tipo póster.*  
*CONGRESS: The 5th International Wilhelm and Else Heraeus Summerschool.*  
*MEETING PLACE: Wittenberg, Alemania.*  
*YEAR: 2-13<sup>th</sup> August 2004.*

---

*AUTHORS: M. Carmen Ruiz Delgado; V. Hernández; R. Ponce Ortiz; J. T. López Navarrete; S. Tanaka; Y. Yamashita.*  
*TITLE: Vibrational and Quantum Chemical Study of Narrow-Bandgap Heterocyclic Cooligomers Containing Alternating Aromatic-Donor and o-Quinoid-Acceptor Units*  
*TYPE OF PRESENTATION: Comunicación tipo póster.*  
*CONGRESS: The 5th International Wilhelm and Else Heraeus Summerschool.*  
*MEETING PLACE: Wittenberg, Alemania.*  
*YEAR: 2-13<sup>th</sup> August 2004.*

---

*AUTHORS: R. Malavé Osuna, R. Ponce Ortiz, M. C. Ruiz Delgado, R. Rathore, V. Hernández, J. T. López Navarrete.*  
*TITLE: FT-IR and FT-Raman Spectroscopic Study aided by DFT Calculations of some  $\pi$ -stacked polyfluorenes.*  
*TYPE OF PRESENTATION: Comunicación tipo póster P4-23.*  
*CONGRESS: XXVII European Congress on Molecular Spectroscopy (EUCMOS 2004)*  
*MEETING PLACE: Cracovia, Polonia*  
*YEAR: 5-10<sup>th</sup> September 2004.*

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*AUTHORS: V. Cuberos Guzmán, R. Ponce Ortiz, M. C. Ruiz Delgado, R. Azumi, R. T. Oakley, J. Casado, V. Hernández, J. T. López Navarrete.*  
*TITLE: FT-IR and FT-Raman Spectroscopic Study, aided by Quantum Chemical DFT Calculations, of a series of oligothiophenes end-capped by nitriles.*  
*TYPE OF PRESENTATION: Comunicación tipo póster P1-39.*  
*CONGRESS: XXVII European Congress on Molecular Spectroscopy (EUCMOS 2004)*  
*MEETING PLACE: Cracovia, Polonia*  
*YEAR: 5-10<sup>th</sup> September 2004.*

---

*AUTHORS: M.C. Ruiz Delgado, F. J. Ramírez, V. Hernández, F. Enríquez and J. T. López Navarrete.*  
*TITLE: Vibrational Dynamics Study of the effect of the Substituents on  $\pi$ -conjugation of Different Bithiophene Molecules.*  
*TYPE OF PRESENTATION: Comunicación tipo póster P1-38.*  
*CONGRESS: XXVII European Congress on Molecular Spectroscopy (EUCMOS 2004)*  
*MEETING PLACE: Cracovia, Polonia*  
*YEAR: 5-10<sup>th</sup> September 2004.*

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*AUTHORS: L. Salford, F. Lubelli, M. Kozaki, V. Hernández, M. C. Ruiz Delgado, R. Ponce Ortiz, J. Casado, J. T. López Navarrete.*

*TITLE: Dímeros de Ciclopentaditiofeno con Bajo Gap Electrónico. Estudio Electroquímico, Raman y Teórico.*

*TYPE OF PRESENTATION: Comunicación Oral.*

*CONGRESS: VII Escuela Nacional de Materiales Moleculares*

*MEETING PLACE: Boí Taüll, Pirineo Catalán, España.*

*YEAR: 29 Marzo -3 Abril 2005.*

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*AUTHORS: M. C. Ruiz Delgado, L. Carrasquer, R. Andreu, J. Orduna, J. Garín, J. Casado, J. T. López Navarrete.*

*TITLE: Análisis Estructural Mediante Espectroscopia IR y Raman y Estudio de las Propiedades Ópticas de una serie de NLO-foros Proaromáticos .*

*TYPE OF PRESENTATION: Comunicación Oral.*

*CONGRESS: VII Escuela Nacional de Materiales Moleculares*

*MEETING PLACE: Boí Taüll, Pirineo Catalán, España.*

*YEAR: 29 Marzo -3 Abril 2005.*

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*AUTHORS: F. Lubelli, L. Salford, P. Bäuerle, P. Frère, V. Hernández, M. C. Ruiz Delgado, R. Ponce Ortiz, J. Casado, J. T. López Navarrete.*

*TITLE: Oligotiofenos Substituidos con Grupos EDO. Estudio Electroquímico, Espectroscópico y Teórico.*

*TYPE OF PRESENTATION: Comunicación Oral.*

*CONGRESS: VII Escuela Nacional de Materiales Moleculares*

*MEETING PLACE: Boí Taüll, Pirineo Catalán, España.*

*YEAR: 29 Marzo -3 Abril 2005.*

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*AUTHORS: R. Ponce Ortiz, R. Malavé Osuna, M. Carmen Ruiz Delgado, J. Casado, V. Hernández, J. Teodomiro López Navarrete, Y. Sakamoto, T. Suzuki.*

*TITLE: Perfluorination of Tetracene: Effects on the Optical Gap and Electron-Acceptor Properties. An Electrochemical, Theoretical DFT, and Raman Spectroscopic Study.*

*TYPE OF PRESENTATION: Comunicación tipo póster [6192-81].*

*CONGRESS: Photonics Europe (An SPIE Europe Event).*

*MEETING PLACE: Strasbourg (France).*

*YEAR: 3-7 Abril 2006.*

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*AUTHORS: R. Malavé Osuna, R. Ponce Ortiz, M. C. Ruiz Delgado, V. Hernández, J. T. López Navarrete, X. Zhang, A. J. Matzger.*

*TITLE: Combined Quantum Chemical DFT, and Spectroscopic Raman and UV-Vis-NIR Study of Fused  $\alpha$ -Oligothiophenes with Five and Seven Rings.*

*TYPE OF PRESENTATION: Comunicación tipo póster [6192-78].*

*CONGRESS: Photonics Europe (An SPIE Europe Event).*

*MEETING PLACE: Strasbourg (France).*

*YEAR: 3-7 Abril 2006.*

---

*AUTHORS: R. Malavé Osuna, M. C. Ruiz Delgado, R. Ponce Ortiz, V. Hernández, J. Casado, J. T. López Navarrete, A. Berlin, G.Zotti.*

*TITLE: Synthesis and Charaterization of a Novel Quinoid Oligothiophene as Electron-donor and Electron-acceptor Material. A Spectroscopic, Electrochemical and Theoretical Study.*

*TYPE OF PRESENTATION: Comunicación tipo póster [P-19].*

*CONGRESS: Trends in Nanoscience: Structure and Functions.*

*MEETING PLACE: Kloster Irsee (Germany).*

YEAR: Octubre 2006.

---

AUTHORS: R. Malavé Osuna, R. Ponce Ortiz, M. C. Ruiz Delgado, V. Hernández, J. T. López Navarrete, X. Zhang, A. J. Matzger.

TITLE: Raman Spectroscopic Analysis and DFT Calculations on Two Fused Thienoacenes with Five and Seven Rings.

TYPE OF PRESENTATION: Comunicación tipo póster [18-W].

CONGRESS: The International Conference on Science and Technology of Synthetic Metals (ICSM 2006).

MEETING PLACE: Dublin (Irlanda).

YEAR: 2-7 Julio 2006.

---

AUTHORS: M. C. Ruiz Delgado, R. Ponce Ortiz, R. Malavé Osuna, J. Casado, V. Hernández, J. T. López Navarrete, Y. Sakamoto and T. Suzuki.

TITLE: Perfluorinated Tetracene: Synthesis, Electrochemistry, Raman Spectroscopic Analysis and DFT Theoretical Calculations.

TYPE OF PRESENTATION: Comunicación tipo póster [19-TU].

CONGRESS: The International Conference on Science and Technology of Synthetic Metals (ICSM 2006).

MEETING PLACE: Dublin (Irlanda).

YEAR: 2-7 Julio 2006.

---

AUTHORS: M.C. Ruiz Delgado, R. Ponce Ortiz, M. Moreno Oliva, J. Casado, V. Hernández, J. T. López Navarrete, E. Ortí, P.M. Viruela, K. Takimiya, T. Otsubo.

TITLE: Physical and Photophysical Studies on Long Quinoidal Oligothiophenes. A Raman Spectroscopic and Theoretical Analysis.

TYPE OF PRESENTATION: Comunicación oral [O-11].

CONGRESS: XX Reunión Nacional de Espectroscopía. IV CONGRESS Ibérico de Espectroscopía.

MEETING PLACE: Ciudad Real.

YEAR: 10-14 Septiembre 2006.

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AUTHORS: R. Malavé Osuna, R. Ponce Ortiz, M. C. Ruiz Delgado, J. Casado, V. Hernández, J.T. López Navarrete, Y. Sakamoto, T. Suzuki.

TITLE: Electrochemical, Theoretical and Raman Spectroscopic Study of Perfluorinated Tetracene.

TYPE OF PRESENTATION: Comunicación tipo póster [PV-104].

CONGRESS: XX Reunión Nacional de Espectroscopía. IV CONGRESS Ibérico de Espectroscopía.

MEETING PLACE: Ciudad Real.

YEAR: 10-14 Septiembre 2006.

---

AUTHORS: M.C. Ruiz Delgado, R. Malavé Osuna, J. Casado, V. Hernández, J.T. López Navarrete, Y. Youichi Sakamoto, S. Komatsu, T. Suzuki, M. Kobayashi, Y. Gao, Y. Fukai, D. A. da Silva Filho, J.L. Brédas.

TITLE: Perfluorination of Tetracene: Raman Study and Charge Transport Properties aided by Quatum-Chemical Calculations.

TYPE OF PRESENTATION: Comunicación oral (Invitada)

CONGRESS: *International Conference of Computational Methods in Sciences and Engineering (ICCMSE).*

MEETING PLACE: *Creta (Grecia).*

YEAR: *27 Octubre-1 Noviembre 2006*

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AUTHORS: *D. A. da Silva Filho, S. Salman, M. C. Ruiz Delgado, J.L. Brédas.*

TITLE: *Charge Transport in Organic Materials.*

TYPE OF PRESENTATION: *Comunicación tipo póster.*

CONGRESS: *The First Solvey-Cope Symposium.*

MEETING PLACE: *Atlanta, GA (USA).*

YEAR: *8 Mayo 2007.*

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AUTHORS: *M.C. Ruiz Delgado, J. Casado, V. Hernandez, J.T. Lopez Navarrete, O.-K. Kim, H. Y. Woo, J. Orduna, B. Villacampa, R. Alicante.*

TITLE: *NLO properties of Dithienothiophene-based chromophores: A comparison study between the Donor/Donor and Donor/Acceptor substitution patterns.*

TYPE OF PRESENTATION: *Comunicación Oral.*

CONGRESS: *SPIE Optics & Photonics.*

MEETING PLACE: *San Diego, California (USA)*

YEAR: *26-30 Agosto 2007.*

---

AUTHORS: *M.C. Ruiz Delgado, R. Malavé Osuna, J. Casado, V. Hernández, J.T. López Navarrete, Y. Youichi Sakamoto, S. Komatsu, T. Suzuki, M. Kobayashi, Y. Gao, Y. Fukai, D. A. da Silva Filho, J.L. Brédas.*

TITLE: *Structure-property Relationships in Perfluorinated Acenes: a Joint Experimental and Theoretical Study.*

TYPE OF PRESENTATION: *Comunicación tipo póster.*

CONGRESS: *Fifth Annual CMDITR Retreat.*

MEETING PLACE: *Atlanta, GA (USA).*

YEAR: *19-21 Febrero 2008.*

---

AUTHORS: *M.C. Ruiz Delgado, R. Malavé Osuna, J. Casado, V. Hernández, J.T. López Navarrete, Y. Youichi Sakamoto, S. Komatsu, T. Suzuki, M. Kobayashi, Y. Gao, Y. Fukai, D. A. da Silva Filho, J.L. Brédas.*

TITLE: *Structure-property Relationships in Perfluorinated Acenes: a Joint Experimental and Theoretical Study.*

TYPE OF PRESENTATION: *Comunicación tipo póster.*

CONGRESS: *The Second Solvey-Cope Symposium.*

MEETING PLACE: *Atlanta, GA (USA).*

YEAR: *6 Mayo 2008.*

---

AUTHORS: *M.C. Ruiz Delgado, D. A. da Silva Filho, J.L. Brédas.*

TITLE: *Tuning Charge Transport Parameters in Perylene Diimide Semiconductors.*

TYPE OF PRESENTATION: *Comunicación tipo póster.*

CONGRESS: *IPRIME Annual Meeting*

MEETING PLACE: *University of Minnesota, Minneapolis, Minnesota (USA).*

YEAR: *27-29 Mayo 2008.*

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*AUTHORS: M.C. Ruiz Delgado, D. A. da Silva Filho, J.L. Brédas.  
TITLE: Tuning Charge Transport Parameters in Perylene Diimide Semiconductors.  
TYPE OF PRESENTATION: Comunicación Oral (Invitada)  
CONGRESS: IPRIME Annual Meeting  
MEETING PLACE: University of Minnesota, Minneapolis, Minnesota (USA).  
YEAR: 27-29 Mayo 2008.*

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*AUTHORS: D. A. da Silva Filho, M.C. Ruiz Delgado, J.L. Brédas.  
TITLE: Charge Transport Properties of Organic Semiconductors: The Case of Perylene Diimides  
TYPE OF PRESENTATION: Comunicación Oral.  
CONGRESS: International Conference on Science and Technology of Synthetic Metals (ICSM 2008).  
MEETING PLACE: Porto de Galinhas, Pernambuco, Brazil.  
YEAR: 6-9 Julio, 2008.*

---

*AUTHORS: M.C. Ruiz Delgado; K. R. Pigg; D.A. da Silva Filho; R.S. Sánchez-Carrera; V. Coropceanu; J.L. Brédas.  
TITLE: Charge-Transport Parameters in the Perfluoropentacene Single Crystal.  
TYPE OF PRESENTATION: Comunicación tipo póster.  
CONGRESS: Gordon Research Conference, Electronic Processes in Organic Materials.  
MEETING PLACE: Mount Holyoke College, South Hadley, MA  
YEAR: 20-25 Julio, 2008.*

---

*AUTHORS: R. Ponce Ortiz; M.C. Ruiz Delgado; J. Casado; V. Hernández; J.T. López Navarrete.  
TITLE: 8th-Spanish National School on Molecular Materials: A Suited Tool To Complement The Scientific Knowledge Of Ph.D. And Master Students In Materials Science.  
TYPE OF PRESENTATION: Comunicación tipo póster.  
CONGRESS: International Conference of Education, Research and Innovation (ICERI 2008).  
MEETING PLACE: Madrid (Spain).  
YEAR: 17-19 Noviembre, 2008*

---

*AUTHORS: R. Ponce Ortiz; M.C. Ruiz Delgado; J. Casado; V. Hernández; J.T. López Navarrete.  
TITLE: Conjugated Organic Molecular Materials: A Suited Research Field For The Training Of Undergraduate Students In Chemistry and Chemical Engineering Into The Learning Of The Materials Science Research.  
TYPE OF PRESENTATION: Comunicación tipo póster.  
CONGRESS: International Conference of Education, Research and Innovation (ICERI 2008).  
MEETING PLACE: Madrid (Spain).  
YEAR: 17-19 Noviembre, 2008*

---

*AUTHORS: M.C. Ruiz Delgado; J.L. Bredas  
TITLE: Tuning Charge-Transport Properties of Organic Semiconductors  
TYPE OF PRESENTATION: Comunicación Oral Invitada.  
CONGRESS: International Workshop on Molecular Materials  
MEETING PLACE: Sanxenxo (Spain).  
YEAR: 2-5 Mayo, 2010*

---

*AUTHORS: M.C. Ruiz Delgado; J.L. Bredas*

*TITLE: Impact of Functionalization on the Charge-Transport Properties of Perylene Diimide Single Crystals*  
*TYPE OF PRESENTATION: Comunicación tipo póster.*  
*CONGRESS: IX Girona Seminar – Electron Density, Density Matrices, and Density Functional Theory*  
*MEETING PLACE: Girona (Spain).*  
*YEAR: 5-8 Julio, 2010*

---

*AUTHORS: M.C. Ruiz Delgado; J.L. Bredas*  
*TITLE: Impact of Functionalization on the Charge-Transport Parameters of Organic Semiconductors.*  
*TYPE OF PRESENTATION: Comunicación tipo póster.*  
*CONGRESS: Ab Initio Modeling in Solid State Chemistry - MSSC2010*  
*MEETING PLACE: London (UK).*  
*YEAR: 13-17 Septiembre, 2010*

---

*AUTHORS: M.C. Ruiz Delgado; J.L. Bredas*  
*TITLE: Tuning the Charge-Transport Parameters of Organic Semiconductors*  
*TYPE OF PRESENTATION: Comunicación Oral.*  
*CONGRESS: VII Simposio de Investigadores Jóvenes Real Sociedad Española de Química-Sigma Aldrich*  
*MEETING PLACE: Valencia (Spain)*  
*YEAR: 10-12 Noviembre 2010*

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*AUTHORS: R. C. González Cano; M. C. Ruiz Delgado; J. Casado; J.T. López Navarrete; Helena Herrera; J.L. Segura*  
*TITLE: Optical and Conformational Properties of a Thiophenic 3D Dendritic Precursor for hyperbranched Polythiophenes*  
*TYPE OF PRESENTATION: Comunicación tipo póster.*  
*CONGRESS: European Conference on Molecular Electronics (ECME)*  
*MEETING PLACE: Barcelona, España*  
*YEAR: 7-10 Septiembre 2011*

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*AUTHORS: R. C. González Cano; J. Casado; M. C. Ruiz Delgado; J.T. López Navarrete; Helena Herrera; J.L. Segura*  
*TITLE: Conformación molecular de oligotiofenos ramificados*  
*TYPE OF PRESENTATION: Comunicación tipo póster.*  
*CONGRESS: VIII Simposio de Investigadores Jóvenes Real Sociedad Española de Química-Sigma Aldrich*  
*MEETING PLACE: Torremolinos, Málaga (Spain)*  
*YEAR: 25-28 Octubre 2011*

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*AUTHORS: R. C. González-Cano; M. C. Ruiz Delgado; J. Casado; J.T. López Navarrete; Helena Herrera; J.L. Segura*  
*TITLE: Estructura electronica de poltiofenos por espectroscopía Raman*  
*TYPE OF PRESENTATION: Comunicación Oral*  
*CONGRESS: Investigadores Jóvenes Real Sociedad Española de Química-Sigma Aldrich*  
*MEETING PLACE: Benicassim, Castellón (Spain)*  
*YEAR: 7-11 Febrero 2011*

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*AUTHORS: J. Casado; Sandra R. González; Rubén Caballero; Pilar de la Cruz; M. Carmen Ruiz Delgado; Juan T. López Navarrete; Fernando Langa*  
*TITLE: Extraordinary long borderline mixed valence systems based on pi-conjugated diferrocenyl thiophene-vinylene oligomers: raman proves a localized-to-delocalized charge transfer excitation*  
*TYPE OF PRESENTATION: Comunicación tipo póster.*  
*CONGRESS: International Symposium on Functional Pi-Electron Systems*  
*MEETING PLACE: Beijing (China)*  
*YEAR: 13-17 Octubre 2011*

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*AUTHORS: J.T. López Navarrete; F.J. Ramírez Aguilar; V. Hernández Jolín; J. Casado Cordón; J.J. Quirante Sánchez; M.C. Ruiz Delgado; R. Ponce Ortiz; M. Moreno Oliva; S. Rodríguez González; C. Capel Ferrón; B. Nieto-Ortega; J.L. Zafra Paredes; R. González Cano; P. Mayorga Burrezo*  
*TITLE: Espectroscopía*  
*TYPE OF PRESENTATION: Comunicación tipo póster.*  
*CONGRESS: I Jornadas de Puertas Abiertas de la Facultad de Ciencias de la Universidad de Málaga "La Química que investigamos"*  
*MEETING PLACE: Málaga (Spain)*  
*YEAR: 27-28 Abril 2011*

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*AUTHORS: R. Juarez; M. Moreno Oliva; M. Ramos; J.L. Segura; M.C. Ruiz Delgado; J. Casado; J.T. López Navarrete*  
*TITLE: HexaAzaTrifenilenos Pi-Extendidos. Nuevos Materiales Aceptores de Electrones*  
*TYPE OF PRESENTATION: Comunicación Oral: C9*  
*CONGRESS: VIII Simposio Investigadores Jóvenes RSEQ Sigma-Aldrich*  
*MEETING PLACE: Torremolinos, Málaga (Spain)*  
*YEAR: 25-28 Octubre 2011*

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*AUTHORS: P. Henrique de Oliveira Neto; Demétrio A. da Silva Filho; M. Carmen Ruiz Delgado; J. Casado; J.T. López Navarrete*  
*TITLE: Structure-Property Relationships on a Terthienoquinoid Derivative: A DFT Study*  
*TYPE OF PRESENTATION: Comunicación tipo póster.*  
*CONGRESS: XVI Simposio Brasileiro de Química Teórica-SBQT 2011*  
*MEETING PLACE: Ouro Preto-MG (Brasil)*  
*YEAR: 20-23 Noviembre de 2011*

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*AUTHORS: W. Ferreira da Cunha; Demétrio A. da Silva Filho; M. Carmen Ruiz Delgado; V. Hernández; J.T. López Navarrete*  
*TITLE: Enhanced Deep-blue Photoluminescence in Thienylene Vinylene Derivatives: A Theoretical Investigation*  
*TYPE OF PRESENTATION: Comunicación tipo póster.*  
*CONGRESS: XVI Simposio Brasileiro de Química Teórica-SBQT 2011*  
*MEETING PLACE: Ouro Preto-MG (Brasil)*  
*YEAR: 20-23 Noviembre de 2011*

---

*AUTHORS: Igor Torres Lima; Demétrio A. da Silva Filho; Berta Gómez-Lor; M. Carmen Ruiz Delgado; J.T. López Navarrete*

*TITLE: Electronic Coupling in Triindole Derivatives: A DFT-D Study*  
*TYPE OF PRESENTATION: Comunicación tipo póster.*  
*CONGRESS: XVI Simposio Brasileiro de Química Teórica-SBOT 2011*  
*MEETING PLACE: Ouro Preto-MG (Brasil)*  
*YEAR: 20-23 Noviembre de 2011*

---

*AUTHORS: M. Carmen Ruiz Delgado; Demétrio A. da Silva Filho; Berta Gómez-Lor; J.T. López Navarrete*  
*TITLE: Electronic and charge-transport properties of Triindoles*  
*TYPE OF PRESENTATION: Comunicación Oral.*  
*CONGRESS: 3<sup>rd</sup> European Symposium on Computing  $\pi$ -Conjugated Systems*  
*MEETING PLACE: Mons (Belgium)*  
*YEAR: 2-4 February de 2012*

---

*AUTHORS: R. C. González-Cano; J. Casado; M. C. Ruiz Delgado; J.T. López Navarrete; Helena Herrera; J.L. Segura*  
*TITLE: Optical and Conformational Properties of a Thiophenic 3D Dendritic Precursor for Hyperbranched Polythiophenes*  
*TYPE OF PRESENTATION: Comunicación tipo póster.*  
*CONGRESS: 3<sup>rd</sup> European Symposium on Computing  $\pi$ -Conjugated Systems*  
*MEETING PLACE: Mons (Belgium)*  
*YEAR: 2-4 February de 2012*

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*AUTHORS: M. Carmen Ruiz Delgado; R. C. González-Cano; J.T. López Navarrete; Helena Herrera; J.L. Segura*  
*TITLE: Flexibility Of Branched Oligothiophenes As Models For 3D Dendritic Polythiophenes*  
*TYPE OF PRESENTATION: Comunicación Oral.*  
*CONGRESS: ICSM 2012 (International Conference on Science and Technology of Synthetic Metals 2012)*  
*MEETING PLACE: Atlanta (USA)*  
*YEAR: 8-13 July 2012*

---

*AUTHORS: M. Carmen Ruiz Delgado; J. T. López Navarrete*  
*TITLE: A Combined Experimental and Theoretical Investigation of the Electronic and Charge-transport Properties of Organic Semiconductors*  
*TYPE OF PRESENTATION: Comunicación Oral Invitada*  
*CONGRESS: IV SEEDMOL*  
*MEETING PLACE: Pirenopolis (Brasil)*  
*YEAR: 24-28 Septiembre de 2012*

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*AUTHORS: M. Carmen Ruiz Delgado; D. Herrero-Carvajal; B. Gómez-Lor; D. A. S. Filho; I. Torres Lima; J. T. López Navarrete*  
*TITLE: Estudio DFT de propiedades electrónicas y de transporte de carga en materiales moleculares basados en la plataforma de triindol*  
*TYPE OF PRESENTATION: Comunicación Oral.*  
*CONGRESS: IX Simposio de Investigadores Jóvenes RSEQ-Sigma Aldrich*  
*MEETING PLACE: Zaragoza (España)*

YEAR: 7-10 Noviembre de 2012

---

AUTHORS: M. Carmen Ruiz Delgado; R. C. González-Cano; J. Casado; J.T. López Navarrete; G. Saini; J. Jacob.

TITLE: Charge Delocalization Study of Branched Oligothiophenes as Models for 3D Dendritic Oligothiophenes

TYPE OF PRESENTATION: Comunicación Oral.

CONGRESS: 4<sup>th</sup> European Symposium on Computing  $\pi$ -Conjugated Systems

MEETING PLACE: Marsella (France)

YEAR: 1-2 February 2013

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AUTHORS: M. C. Ruiz Delgado; R. C. González-Cano; G. Saini; J. Jacob; J. Casado; J.T. López Navarrete

TITLE: Flexibility of Ramified Oligothiophenes in their Neutral and Oxidized States

TYPE OF PRESENTATION: Comunicación Oral.

CONGRESS: XXIX Congreso Internacional de Químicos Teóricos de Expresión Latina

MEETING PLACE: Granada (España)

YEAR: 30 Junio-5 Julio de 2013

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AUTHORS: M. Carmen Ruiz Delgado; Rafael C. González Cano; Juan Casado; J.T. López Navarrete

TITLE: Estudio de Estados Excitados y Deslocalización de Carga en Oligotiofenos Ramificados

TYPE OF PRESENTATION: Comunicación Oral.

CONGRESS: XXXIV Reunión Bienal de la Real Sociedad Española de Química

MEETING PLACE: Santander (España)

YEAR: 15-18 Septiembre de 2013

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AUTHORS: M. Carmen Ruiz Delgado; C. Capel Ferrón; M. Capdevila-Cortada; Juan J. Novoa; V. Hernández; J.T. López Navarrete

TITLE: *II*-Dimerización de Especies Oxidadas en Oligotiofenos Fusionados

TYPE OF PRESENTATION: Comunicación póster.

CONGRESS: XXXIV Reunión Bienal de la Real Sociedad Española de Química

MEETING PLACE: Santander (España)

YEAR: 15-18 Septiembre de 2013

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AUTHORS: M. Carmen Ruiz Delgado; C. Capel Ferrón; M. Capdevila-Cortada; Juan J. Novoa; V. Hernández; J.T. López Navarrete

TITLE: *II*-Dimerización de Especies Oxidadas en Oligotienoacenos

TYPE OF PRESENTATION: Comunicación Oral.

CONGRESS: X Simposio de Investigadores Jóvenes RSEQ-2013

MEETING PLACE: Madrid (España)

YEAR: 6-9 Noviembre 2013

---

AUTHORS: M. Carmen Ruiz Delgado; C. Capel Ferrón; M. Capdevila-Cortada; Juan J. Novoa, F. Hartl; V. Hernández; J. T. López Navarrete

TITLE:  $\pi$ -Dimerization of Heptathienoacene Radical Cations

TYPE OF PRESENTATION: Comunicación Oral.

CONGRESS: 5<sup>th</sup> European Symposium on Computing  $\pi$ -Conjugated Systems

MEETING PLACE: Linköping (Sweden)

YEAR: 5-7 February 2014

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*AUTHORS: M. Carmen Ruiz Delgado, D. Herrero-Carvajal, G.L. Gibson, D.S. Seferos, J.T. López Navarrete*

*TITLE: Tuning the Electronic Properties in Benzochalcogenodiazole-Based D–A Type Copolymers by Heteroatom Substitution*

*TYPE OF PRESENTATION: Comunicación Oral.*

*CONGRESS: 6<sup>th</sup> European Symposium on Computing  $\pi$ -Conjugated Systems*

*MEETING PLACE: Olomouc (Czech Republic)*

*YEAR: 5-7 February 2014*

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*AUTHORS: M. Carmen Ruiz Delgado; C. Capel Ferrón; M. Capdevila-Cortada; Juan J. Novoa, F. Hartl; V. Hernández; J. T. López Navarrete*

*TITLE:  $\pi$ -Dimerization of Heptathienoacene Radical Cations*

*TYPE OF PRESENTATION: Comunicación Oral.*

*CONGRESS: 5<sup>th</sup> European Symposium on Computing  $\pi$ -Conjugated Systems*

*MEETING PLACE: Linköping (Sweden)*

*YEAR: 5-7 February 2014*

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*AUTHORS: Víctor Hernández, Cristina Capel Ferrón, Rocío Ponce Ortiz, M. Carmen Ruiz Delgado, Juan T. López Navarrete, Christine K. Luscombe, Lauren J. Kang, Katherine A. Mazzio*

*TITLE: Raman spectroscopic study of regioregular poly(3-alkylthiophene)s with low dispersity obtained through external initiation polymerization*

*TYPE OF PRESENTATION: Poster.*

*CONGRESS: 12<sup>th</sup> International Symposium on Functional  $\pi$ -Electron Systems (F $\pi$ -12)*

*MEETING PLACE: University of Washington, Seattle, USA*

*YEAR: July 19-24, 2015*

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*AUTHORS: M. Carmen Ruiz Delgado, C. Capel Ferrón, M. Capdevila-Cortada, Juan J. Novoa, F. Hartl, V. Hernández, J. T. López Navarrete*

*TITLE:  $\pi$ -Dimerization of Oligothienoacene Radical Cations*

*TYPE OF PRESENTATION: Oral communication*

*CONGRESS: 12<sup>th</sup> International Symposium on Functional  $\pi$ -Electron Systems (F $\pi$ -12)*

*MEETING PLACE: University of Washington, Seattle, USA*

*YEAR: July 19-24, 2015*

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*AUTHORS: M. Carmen Ruiz Delgado, C. Capel Ferrón, M. Capdevila-Cortada, Juan J. Novoa, F. Hartl, V. Hernández, J. T. López Navarrete*

*TITLE:  $\pi$ -Dimerization of Fused Oligothiophene Radical Cations*

*TYPE OF PRESENTATION: Poster.*

*CONGRESS: Molecular Simulation and Engineering Conference, MolSimEng 2015*

*MEETING PLACE: Politecnico di Milano, Milan (Italy)*

*YEAR: September 18 2015*

---

*AUTHORS: M. Carmen Ruiz Delgado, C. Capel Ferrón, V. Hernández, J.T. López Navarrete, L. Brambilla, M. Tommasini, A. Milani, C. Castiglioni, K. Sugiyasu*

*TITLE: Investigation of the Long Effective Conjugation Length in Defect-Free Insulated Molecular Wires*

*TYPE OF PRESENTATION: Oral.*

*CONGRESS: 7<sup>th</sup> European Symposium on Computing  $\pi$ -Conjugated Compounds MEETING PLACE: Bordeaux (France)*

*YEAR: February 12-13th, 2015*

## MASTER (DEA) SUPERVISED

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*TITLE: Oligotiofenos pro-dendriméricos: Espectroscopía Raman Resonante y química Cuántica*

*Ph. D. STUDENT: Rafael C. González Cano*

*UNIVERSITY: University of Málaga*

*FACULTY/SCHOOL: Faculty of Sciences*

*YEAR: September, 2011*

*MARK: Outstanding Mention*

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*TITLE: Efecto de una sustitución monoatómica en polímeros Dador-Aceptor para Electrónica Orgánica.*

*Ph. D. STUDENT: Daniel Herrero Carvajal*

*UNIVERSITY: University of Málaga*

*FACULTY/SCHOOL: Faculty of Sciences*

*YEAR: July, 2013*

*MARK: Outstanding Mention*

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## BACHELOR THESES SUPERVISED

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*TITLE: Polímeros de Fenileno y Tiofenos con Electro-aceptores periféricos. Estudio por espectroscopías Raman y electrónica y Modelización Molecular.*

*Ph. D. STUDENT: Daniel Herrero Carvajal*

*UNIVERSITY: University of Málaga*

*FACULTY/SCHOOL: Faculty of Sciences*

*YEAR: Julio, 2012*

*MARK: Outstanding Mention*

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*TITLE: Modulación de las Propiedades Ópticas y Electrónicas en Polímeros Biaxiales para Electrónica Orgánica*

*Ph. D. STUDENT: Leticia Ruiz Castillo*

*UNIVERSITY: University of Málaga*

*FACULTY/SCHOOL: Faculty of Sciences*

*YEAR: Diciembre, 2013*

*MARK: Outstanding Mention*

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## PhD SUPERVISED

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*TITLE: Study of Inter- and Intramolecular Electronic Properties of Oligothiophenes and Heteroaromatic Polymers*

*Ph. D. STUDENT: Cristina Capel Ferrón*

*UNIVERSITY: University of Málaga*

*FACULTY/SCHOOL: Faculty of Sciences*

*YEAR: Defended with honors in December 3th, 2013*

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*TITLE: Charge Delocalization of branched oligothiophenes for organic electronics.*

*Ph. D. STUDENT: Rafael Carlos González Cano*

*UNIVERSITY: University of Málaga*

*FACULTY/SCHOOL: Faculty of Sciences*

*YEAR: Currently under supervision*

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## REFEREE RESEARCHERS

(Up to 3 researchers' names may be given by applicant to give references.  
Compliance of this section is not compulsory for the applicant)

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*SURNAMES, NAME: Prof. Dr. Jean-Luc Brédas*

*PROFESSIONAL RELATIONSHIP WITH APPLICANT: Research Director  
(Professor-tutor, Research director, Employee-boss, Collaborator, Others)*

*LENGTH OF RELATIONSHIP (give dates): Postdoctoral period Supervisor (from 01/04/2007, at present);  
Supervisor during a PhD visiting stay (September-December 2005)*

*BODY TO WHICH YOU BELONG TODAY: School of Chemistry and Biochemistry, and Center for  
organic Photonics and Electronics. Georgia Institute of Technology, Atlanta, USA.  
(Institution and country)*

*POST: Professor and Chair in Molecular Design. Georgia Alliance Eminent Scholar.*

*TELEPHONE: (001) 404-385-4986*

*E-MAIL: jean-luc.bredas@chemistry.gatech.edu*

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*SURNAMES, NAME: Dr. Slava Coropceanu*

*PROFESSIONAL RELATIONSHIP WITH APPLICANT: Collaborator  
(Professor-tutor, Research director, Employee-boss, Collaborator, Others)*

*LENGTH OF RELATIONSHIP (give dates): From 01/04/2007, at present*

*BODY TO WHICH YOU BELONG TODAY: School of Chemistry and Biochemistry, and Center for  
organic Photonics and Electronics. Georgia Institute of Technology, Atlanta, USA.  
(Institution and country)*

*POST: Principal Research Scientist*

*TELEPHONE: (001)404-385-8181*

*E-MAIL: coropceanu@chemistry.gatech.edu*

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*SURNAMES, NAME: Dr. Jesús Orduna Catalán*

*PROFESSIONAL RELATIONSHIP WITH APPLICANT: Research director  
(Professor-tutor, Research director, Employee-boss, Collaborator, Others)*

*LENGTH OF RELATIONSHIP (give dates): Supervisor during postdoctoral (January-March 2007) and  
PhD visiting stays (July-October 2004)*

*BODY TO WHICH YOU BELONG TODAY: Institute of Materials Science of Aragón  
(Institution and country)*

*POST: CSIC Principal Researcher Scientist*



TELEPHONE: 976-761194

E-MAIL: jorduna@unizar.es

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*SURNAMES, NAME: Dr. Javier Garín Tercero*

*PROFESSIONAL RELATIONSHIP WITH APPLICANT: Research director  
(Professor-tutor, Research director, Employee-boss, Collaborator, Others)*

*LENGTH OF RELATIONSHIP (give dates): Supervisor during postdoctoral (January-March 2007) and  
PhD visiting stays (July-October 2004)*

*BODY TO WHICH YOU BELONG TODAY: Institute of Materials Science of Aragón and Universidad de  
Zaragoza  
(Institution and country)*

*POST: Full Professor Universidad de Zaragoza*

TELEPHONE: 976-761194

E-MAIL: jgarin@unizar.es

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*SURNAMES, NAME: Dr. Juan Teodomiro López Navarrete*

*PROFESSIONAL RELATIONSHIP WITH APPLICANT: Research director  
(Professor-tutor, Research director, Employee-boss, Collaborator, Others)*

*LENGTH OF RELATIONSHIP (give dates): Ph.D. Supervisor and current group leader*

*BODY TO WHICH YOU BELONG TODAY: Universidad de Málaga  
(Institution and country)*

*POST: Full Professor*

TELEPHONE: 952-132018

E-MAIL: teodomiro@uma.es

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## Participation in International Committees and Representations

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Committee Title: Peer Reviewer

Entity: Elsevier (Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy)

Subject: Peer Reviewing

Year: Since 2011

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Committee Title: Peer Reviewer

Entity: Elsevier (Food Chemistry)

Subject: Peer Reviewing

Year: Since 2013

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Committee Title: Peer Reviewer

Entity: acs publications (Journal of Physical Chemistry)

Subject: Peer Reviewing

Year: Since 2013

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Committee Title: Peer Reviewer

Entity: Royal Society of Chemistry (Physical Chemistry Chemical Physics)

Subject: Peer Reviewing

Year: Since 2014

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Committee Title: Reviewer

Entity: Agencia Nacional de Evaluación y Prospectiva (ANEP)

Subject: Peer Reviewing of National Projects

Year: Since 2011

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Committee title: Grupo especializado de Jóvenes Químicos de la Real Sociedad Española de Química

Organization which runs it: Real Sociedad Española de Física y Real Sociedad Española de Química

Issue: Member of the board, treasurer

Year: Since 2013

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Committee title: Grupo especializado de Jóvenes Químicos de la Real Sociedad Española de Química

Organization which runs it: Real Sociedad Española de Física y Real Sociedad Española de Química

Issue: Member of the board, Vicepresident

Year: Since 2010

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Committee title: Junta de Centro

Organization which runs it: Faculty of Sciences (University of Málaga)

Issue: Member of the board

Year: Since 2010

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Committee title: Claustro Universitario

Organization which runs it: Faculty of Sciences (University of Málaga)

Issue: Member of the board

Year: Since 2010

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**Experience in the Organization of R&D activities**  
Organization of Conferences, Seminars, etc

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**Conferences**

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Conference Title: VIII Simposio de Investigadores Jóvenes RSEQ-Sigma Aldrich, Torremolinos (Málaga)

Activity Type: Scientific Organizer

Date: 25-28 Octubre 2011

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## Schools

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Conference Title: VIII Escuela Nacional de Materiales Moleculares 2007, Estepona (Málaga)

Activity Type: Scientific Organizer

Date: 20-27 Mayo 2007

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### OTHER ACHIEVEMENTS (in one DIN A4 page only)

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- **SCIENTIFIC AWARDS:**

- 2010, RSEQ (Spanish Royal Society Academy of Chemistry) and Sigma-Aldrich Young Investigator Award.
- 2010, Atlanta Area Chemical Physics Postdoctoral Award. This Award recognizes excellence in research and is coordinated jointly between the two main Universities in Georgia (USA): Georgia Tech and Emory University.
- 2007, Fundación General de la Universidad de Málaga Young Investigator Award.
- 2007, Dr. Esteban Pérez-Bryan Souvirón Award for the best Ph.D. Thesis in Chemistry, University of Málaga and University of Granada.
- 2007, RSEQ (Spanish Royal Society Academy of Chemistry) Award for the best Ph.D. Thesis in Nanoscience and Molecular Materials.
- 2007, University of Málaga Award for the best Ph.D. Thesis in Chemistry

- **TEACHING EXPERIENCE:**

- Instructed and coordinator of the General Chemistry Course of Industrial Electronic Engineer Undergraduate for the academic year: 2011/2012. Total Hours: 60 hours. Place: Physical Chemistry Department, University of Málaga.
- Instructed the physical chemistry laboratory for the following years (60 hours/academic year): 2009/2010, 2011/2012. Total Hours: 120 hours. Place: Physical Chemistry Department, University of Málaga.
- Instructed the physical chemistry laboratory for the following years (during the PhD period): 2004/2005; 2005/2006; 2007/2008. Total Hours: 120 hours. Place: Physical Chemistry Department, University of Málaga.
- Participation in a Research Project devoted to Innovation in Education:
  - Title: "Diseño de Actividades On-line Orientadas a la Enseñanza Experimental en Química Física". Vicerrectorado de Ordenación Académica y Profesorado de la Universidad de Málaga. Period :2010/2012
- Attendance to different conferences/courses on didactics and Education:
  - "Curso de Formación para el Profesorado Universitario Novel". Place: University of Málaga. Year: 2004/2005
  - CAP (Curso de Adaptación Pedagógica). Place: University of Málaga. Year :2001/2002

- **PROFESSIONAL SKILLS:**

- Acquainted with scientific software such as ADF, Gaussian, Turbomole, Material Studio, Jaguar, Crystal.
- Acquainted in visualization programs such as Molden, Molekel, Xcryden, ZOA, Moldraw.
- Proficiency in UNIX operating systems and conversant in computers.
- Experience with using the Cambridge Structural Database.