# Currículum vítae

Nombre: María del Carmen Ruiz Delgado

Fecha: 11-09-2014

Family name: Ruiz Delgado	Forename: Mª del Carmen		
ID/Passport no: 77469096-J Nacionality: Spain	Date of birth : May 7, 1977	7 Gender: H	emale
PRES	ENT PROFESIONAL POS	ITION	
Institution: University of Málaga Faculty, School or Institute: Faculty of S Department: Department of Physical Cl Address: Campus de Teatinos Post Cod: 29071 Province: Málaga Country: Spain	Science hemistry		
Telephone (indicate prefix, number and Fax: - E-mail: carmenrd@uma.es	l extension): 952-131863		
Field of study (UNESCO codes): Main	Field: 23; Subfields: 2306.1	0, 2211.09, 2210.20, 220	6.08, 2206.09,
Profesional status: Ramón y Caja Fellow	I Research	Start date: November 1	9, 2010
Administrative status	Hired on contracts	Acting	
Full-time 🔀 Part-time 🗌			

### 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.

### ACADEMIC BACKGROUND

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

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

### PAST SCIENTIFIC EXPERIENCE (\*)

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

(\*) 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)

Language	Speaking	Reading	Writing
English	G	Р	Р
German	Ν	Ν	Ν

### PARTICIPATION IN RESEARCH PROJECTS (limited to 2012-2014)

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

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-Oligothienylene-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

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 and 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

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

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, and 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

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 (\*):

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 (\*):

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

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

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

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, and 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-ethylenenedioxyselenophene)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): Martin Scheuble, Thomas V. Richter, Miriam Goll, Steffen Link, Juan T. López Navarrete, Adrian Ruff, M. Carmen Ruiz Delgado and Sabine Ludwigs

TITLE: Branched polythiophenes by Ni-catalyzed Kumada coupling

JOURNAL/BOOK TITLE: Polym. Chem. (accepted) DOI: 10.1039/C4PY00899E 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)

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 solidstate 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.

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.

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.

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 knowledege). 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.

### STAYS IN INTERNATIONALLY RECOGNIZED CENTRES

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

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

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

CENTRE: School of Chemistry and Biochemistry. Georgia Institute of TechnologyPLACE:AtantaCOUNTRY: USAYEAR: 2005LENGHT: 16 weeksTOPIC: Charge-transport properties in Organic SemiconductorsKEY: DSupervisor: Prof. Dr. Jean-Luc BrédasKEY: D

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

CENTRE: School of Chemistry and Biochemistry. Georgia Institute of Technology PLACE:Atanta 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

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

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

### PRESENTATIONS IN CONGRESSES (Limited to 2012-2014)

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: ADFT-D 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

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:  $3^{rd}$  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:  $3^{rd}$  European Symposium on Computing  $\pi$ -Conjugated Systems MEETING PLACE: Mons (Belgium) YEAR: 2-4 February de 2012

AUTHORS: M. Carmen Ruiz Delgado, Demétrio A. da Silva Filho, Berta Gómez-Lor, J.T. López Navarrete 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 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

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

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

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

AUTHORS: M. Carmen Ruiz Delgado, C. Capel Ferrón, M. Capdevila-Cortada, Juan J. Novoa, V. Hernández, J.T. López Navarrete TITLE: IT-Dimerización de Especies Oxidadas en Oligotienoacenos TYPE OF PRESENTATION: Comunicación Oral. AUTHORS: M. Carmen Ruiz Delgado, C. Capel Ferróna, 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

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

### • 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/curses 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.