



CURRICULUM VITAE (CVA)

IMPORTANT – The Curriculum Vitae cannot exceed 4 pages. Instructions to fill this document are available in the website.

Part A. PERSONAL INFORMATION

CV date 11/05/2023

First name	Enrique		
Family name	Ortí Guillén		
Gender (*)	Male	Birth date	
Social Security, Passport, ID number			
e-mail	enrique.orti@uv.es	URL Web	
Open Researcher and Contributor ID (ORCID) (*)	0000-0001-9544-8286		

(*) Mandatory

A.1. Current position

Position	Catedrático (Full Professor)		
Initial date	08/07/2008		
Institution	Universidad de Valencia		
Department/Center	Instituto de Ciencia Molecular	Departamento de Química Física	
Country	Spain	Teleph. number	+34 963544438
Key words	Computational chemistry, molecular materials, organic semiconductors, electroluminescence, fullerenes, supramolecular aggregates and polymers, energy and charge transfer.		

A.2. Previous positions (research activity interruptions, art. 14.2.b))

Period	Position/Institution/Country/Interruption cause
March 1987 – July 2008	Associate Prof. (Prof. Titular) / Univ. Valencia / Spain
Oct. 1986 – March 1987	Assistant (Ayudante LRU) / Univ. Valencia / Spain
Feb. 1986 – Sept. 1986	Assistant / Univ. Valencia (Colegio Univ. Castellón) / Spain
January 1982 – Dec. 1985	Predoctoral fellow / Univ. Valencia / Spain

A.3. Education

PhD, Licensed, Graduate	University/Country	Year
Licensed in Chemical Sciences	Universidad de Valencia / Spain	1979
PhD in Chemical Sciences	Universidad de Valencia / Spain	1985

Part B. CV SUMMARY (max. 5000 characters, including spaces)

Enrique Ortí obtained his Ph.D. degree in Chemistry with academic honors from the Univ. of Valencia in 1985 under the supervision of Profs. F. Tomás and J. Sánchez-Marín. In 1987, he did a postdoctoral stay with Prof. J.-L. Brédas (Laboratoire de Chimie Théorique Appliquée, Univ Namur, Belgium), where he worked on the calculation of periodic systems (conjugated polymers and aggregates). He became Assistant and Associate Professor in Physical Chemistry at the University of Valencia in 1986 and 1987, respectively. Since 2008, he is Full Professor of Physical Chemistry at this university.

E. Ortí is research member of the Institute of Molecular Science (ICMol) of the University of Valencia, which has been distinguished two times with the accreditation as a *Unit of Excellence "Maria de Maeztu"*, where he leads the Molecular Materials Theoretical Chemistry Group (MolMatTC, <http://www.uv.es/qcmatmol/>) since its foundation in 1988. His main interests concern the theoretical characterization of functional electroactive/photoactive molecular

materials of special relevance in the field of *Molecular Electronics*. The MolMatTC group, under the leadership of Dr. E. Ortí, has collaborated with many Spanish and international research groups involved in the synthesis, characterization and device development of molecular materials. The results obtained have been of special relevance for: 1) optimizing the photophysical properties of luminescent materials used in light-emitting devices (LECs and OLEDs), 2) understanding the charge transfer processes of electron donor/acceptor systems used in solar cells, 3) disentangling the structural and energetic aspects of molecular aggregation phenomena and supramolecular polymer formation, and 4) predicting the charge and energy transport properties of new organic semiconductors. E. Ortí was one of pioneers of the scientific community working on molecular materials currently grouped in the multidisciplinary RSEQ/RSEF group of Nanoscience and Molecular Materials (Nanomatmol).

E. Ortí has published 332 papers (134 (106 in Q1) in the period 2013-2023,), many of them in high-impact multidisciplinary chemistry journals (see **C.1**), which accumulate 11738 citations and have an average number of citations of 37 (***h index* 59**). He has been involved in 37 research projects (24 as principal investigator, 3 excellence PROMETEO projects) and has participated in 4 European Projects. He has given around 125 invited/plenary talks and seminars (74 in the period 2013-2023) and has been Visiting Professor of the Univ. of Mons (Belgium). In 2014, he was distinguished with the *Award to the Research Excellence of the Spanish Royal Society of Chemistry* (RSEQ).

E. Ortí has supervised 17 Doctoral Thesis (11 in the last 10 years), one of them awarded with the *2011 IUPAC Prize for Young Chemists*, 4 with the *Premio Extraordinario de Doctorado en Química* and 4 received the *Nanomatmol Doctorate Award*. 10 of these students have continued a scientific career in Universities or Research Centers (Universidad de Valencia, Technical University of Munich, Universidad de Zaragoza), 1 has obtained an ERC contract, and 3 of them enjoy excellence research contracts (Ramón y Cajal, Juan de la Cierva and CDEIGENT). He actively participates in the Erasmus Mundus Master on Theoretical Chemistry and Computational Modelling, and is the coordinator at the Universidad de Valencia of the Doctoral Program on Theoretical Chemistry and Computational Modelling. E. Ortí has organized two Molecular Materials National Schools (ENMM-2001 and 2015) and is largely involved in the scientific symposium and the informative open-doors activities organized annually by the ICMol.

Part C. RELEVANT MERITS (*sorted by typology*)

C.1. Publications

Author of **134 papers** in the period 2013-2023: **106** (78%) are ranked in the first quartile (**Q1**), **24** in journals with **IF >15**, **20** with **IF** between **9** and **15**, **58** with **IF** between **4** and **9**.

Multidisciplinary Chemistry (**50**): **9** in *JACS*, **7** in *Angew. Chem. Int. Ed.*, **6** in *Chem. Sci.*, **4** in *Chem. Commun.*, **14** in *Chem. Eur. J.*, **10** in other journals.

Materials Chemistry (**40**): **1** in *Nature Photon.*, **2** in *Adv. Mater.*, **2** in *Adv. Energy Mater.*, **1** in *Adv. Funct. Mater.*, **1** in *Small*, **2** in *ACS Appl. Mater. Interfac.*, **5** in *Chem. Mater.*, **18** in *J. Mater. Chem. A* and *C*, **2** in *Solar RRL*, **5** in other journals.

Physical (**5**), Inorganic (**7**) and Organic (**2**) Chemistry. Book Chapters (**2**).

1. M. Vicent-Morales, M. Esteve-Rochina, J. Calbo, E. Ortí, I. J. Vitórica, G. Mínguez, "Semiconductor Porous Hydrogen-Bonded Organic Frameworks Based on Tetrathiafulvalene Derivatives" *J. Am. Chem. Soc.* **2022**, *144*, 9074–9082. (Impact factor (IF): **16.383**)
2. S. Bujosa, A. Doncel-Giménez, N. Bäumer, G. Fernández, E. Ortí, A. Costa, C. Rotger, J. Aragó, B. Soberats, "Thermoreversible Polymorph Transitions in Supramolecular Polymers of Hydrogen-Bonded Squaramides" *Angew. Chem. Int. Ed.* **2022**, *61*, e202213345 (8 pp). (IF: **16.823**).
3. M. A. Martínez, A. Doncel-Giménez, J. Cerdá, J. Calbo, R. Rodríguez, J. Aragó, J. Crassous, E. Ortí, L. Sánchez, "Distance Matters: Biasing Mechanism, Transfer of Asymmetry, and Stereomutation in N-Annulated Perylene Bisimide Supramolecular Polymers"

- J. Am. Chem. Soc.* **2021**, *143*, 13281–13291. (Impact factor (IF): **16.383**).
4. R. Caballero, M. Barrejón, J. Cerdá, J. Aragón, S. Seetharaman, P. de la Cruz, E. Ortí, F. D'Souza, F. Langa, "Self-Assembly-Directed Organization of a Fullerene–Bisporphyrin into Supramolecular Giant Donut Structures for Excited-State Charge Stabilization" *J. Am. Chem. Soc.* **2021**, *143*, 11199–11208. (IF: **16.383**).
 5. M. J. Mayoral, J. Calbo, J. Aragón, F. Aparicio, E. Ortí, T. Torres, D. González-Rodríguez, "Dual-Mode Chiral Self-Assembly of Cone-Shaped Subphthalocyanine Aromatics" *J. Am. Chem. Soc.* **2020**, *142*, 21017–21031. (IF: **16.383**, Citations: **17**).
 6. E. E. Greciano, J. Calbo, E. Ortí, L. Sánchez, "N-Annulated Perylene Bisimides to Bias the Differentiation of Metastable Supramolecular Assemblies into J- and H-Aggregates" *Angew. Chem. Int. Ed.* **2020**, *59*, 17517–17524. (IF: **16.823**, Citations: **37**).
 7. E. E. Greciano, J. Calbo, J. Buendía, J. Cerdá, J. Aragón, E. Ortí, L. Sánchez, "Decoding the Consequences of Increasing the Size of Self-Assembling Tricarboxamides on Chiral Amplification" *J. Am. Chem. Soc.* **2019**, *141*, 7463–7472. (IF: **16.383**, Citations: **33**).
 8. I. García-Benito, I. Zimmermann, J. Urieta-Mora, J. Aragón, J. Calbo, J. Perles, A. Serrano, A. Molina-Ontoria, E. Ortí, N. Martín, M. K. Nazeeruddin, "Heteroatom Effect on Star-Shaped Hole-Transporting Materials for Perovskite Solar Cells" *Adv. Funct. Mater.* **2018**, *28*, 1801734. (IF: **19.954**, Citations: **58**).
 9. M. Souto, J. Romero, J. Calbo, I. J. Vitorica-Yrezabal, J. L. Zafra, J. Casado, E. Ortí, A. Walsh, G. Mínguez-Espallargás, "Breathing-Dependent Redox Activity in a Tetrathiafulvalene-Based Metal–Organic Framework" *J. Am. Chem. Soc.* **2018**, *140*, 10562–10569. (IF: **16.383**, Citations: **50**).
 10. I. Zimmermann, J. Urieta-Mora, P. Gratia, J. Aragón, G. Grancini, A. Molina-Ontoria, E. Ortí, N. Martín, M. K. Nazeeruddin, "High-Efficiency Perovskite Solar Cells using Molecularly-Engineered, Thiophene-Rich, Hole-Transporting Materials" *Adv. Energy Mater.* **2017**, *7* (6), 1601674 (1-8). (IF: **29.698**, Citations: **118**).

C.2. Congresses

Invited, keynote or contributed lectures in congresses: 85 (45 in the period 2013-2023)

Invited talks in research centers and universities: 50 (26 in the period 2013-2023)

1. E. Ortí (Invited lecture), *Ionic Transition-Metal Complexes for Light-Emitting Electrochemical Cells: A Theoretical Insight*, 3rd International Symposium on Molecular Design of Optoelectronic Materials, Beijing (China), 24-26 May 2019.
2. E. Ortí (Invited lecture), *A Theoretical Insight into the Self-Assembly of Electroactive Systems: From Dimers to Supramolecular Polymers*, Molecular Design of Organic Optoelectronic Materials, Beijing (China), 21-23 May 2019.
3. E. Ortí (Invited lecture), *Self-Assembly of Electroactive Systems: From Dimers to Supramolecular Polymers*, 10th Symposium on Computing π -Conjugated Compounds, Valencia (Spain), 31 January – 2 February 2019.
4. E. Ortí (Invited lecture), *Hole transporting materials for perovskite solar cells: A theoretical insight*, XI European School on Molecular Nanoscience (ESMOLNA 2018), Puerto de Santiago, Tenerife (Spain), 20-25 May 2018.
5. E. Ortí (Invited lecture), *Theoretical approach to the supramolecular organization of electroactive molecular systems*, XVII National School on Molecular Materials (XVII ENMM), Torremolinos (Spain), 11-15 February 2018.
6. E. Ortí (Contributed talk), *Ionic Ir(III) Complexes as Electroluminescent Materials for Light-Emitting Devices: Emission Color and Efficiency*, 6th EuCheMS Chemistry Congress, Sevilla (Spain), 11 – 15 September 2016.
7. E. Ortí (Invited lecture), *Supramolecular Organization of Electroactive Molecular Systems: A Theoretical Insight*, POLYMAT Spotlight, San Sebastián (Spain), 21-24 June 2016.

8. E. Ortí (Invited lecture), *Supramolecular Organization of Electroactive Molecular Systems*, VIII European School on Molecular Nanoscience (ESMOLNA 2015), Paris (France), 25-29 October 2015.
9. E. Ortí (Contributed talk), *Concave Donors as Supramolecular Partners for Fullerene C₆₀*, 16th International Symposium on Novel Aromatic Compounds (ISNA16), Madrid (Spain), 5-10 July 2015.
10. E. Ortí (Invited lecture), *Donor-Acceptor Supramolecular Associates Involving Fullerene C₆₀*, XI Girona Seminar on Carbon, Metal, and Carbon-Metal Clusters: From Theory to Applications, Girona (Spain), 30 June – 3 July 2014.

C.3. Research projects

Member of the research team in 37 research projects, 24 as principal investigator

1. *Modelización computacional de materiales moleculares electroactivos: estructura electrónica, organización supramolecular y propiedades de transporte*, MCIN (PID2021-128569NB-I00), Sept. 2022 - Agosto 2025, 175.450 €, **PI**: E. Ortí.
2. *Modelización computacional de materiales funcionales inteligentes para electrónica molecular*, Generalitat Valenciana (**MFA/2022/017**), Jul. 22 - Jun. 25, 144.559 €, **PI**: E. Ortí.
3. *Materiales disruptivos foto/electroactivos para células solares de perovskita híbridas 2D de alta estabilidad*, MCIN (TED2021-131255B-C44), Dic. 22 - Nov. 24, 172.500 €, **PI**: E. Ortí.
4. *Desarrollo de nuevos semiconductores y su uso en dispositivos emisores de luz y células solares.*, Generalitat Valenciana (PROMETEO/2020/077), Sept. 2020 - Dec. 2023, 216.525 €, **PI**: E. Ortí.
5. *Estructura electrónica, organización supramolecular y propiedades de transporte de materiales moleculares electroactivos*, MCIN/AEI (PGC2018-099568-B-I00), January 2019 – Dec. 2021, 121.000,00 €, **PI**: E. Ortí.
6. *Sistemas Electroactivos para Electrónica Molecular: Dispositivos Emisores de Luz y Fotovoltaicos Eficientes.*, Generalitat Valenciana (PROMETEO/2016/135), Sept. 2016 - Dec. 2019, 205.973 €, **PI**: E. Ortí.
7. *Sistemas moleculares electroactivos: Estructura electrónica, propiedades ópticas y organización supramolecular*, MINECO (CTQ2015-71154-P), Enero 2016 – Dic. 2018, 92.100,00 €, **PI**: E. Ortí.
8. *Estudio Teórico de Sistemas Electroactivos/Fotoactivos para Electrónica Molecular*, MINECO (CTQ2012-31914), January 2013 – Dec. 2015, 89.000,00 €, **PI**: E. Ortí.
9. *Dispositivos Moleculares Emisores de Luz y Fotovoltaicos*, Generalitat Valenciana (PROMETEO/2012/053), June 2012 - Dec. 2015, 193.521 €, **PI**: E. Ortí.
10. *Hybrid Molecule-Nanocrystal Assemblies for Photonic and Electronic Sensing Applications* European Union (FP7-263091), Abril 2011 - Marzo 2014, 258.527 €, **PI**: H. J. Bolink

C.4. Contracts, technological or transfer merits

1. *María de Maeztu Excellence Unit - Instituto de Ciencia Molecular*, MCIN/AEI (CEX2019-000919-M), Jan. 2020 - Dec. 2023, 2.000.000 €, **IP**: E. Coronado, E. Ortí (group leader).
2. *María de Maeztu Excellence Unit - Instituto de Ciencia Molecular*, MINECO (MDM-2015-0538), Jan. 2016 - Dec. 2019, 2.000.000 €, **IP**: E. Coronado, E. Ortí (GL: group leader).
3. *Functional Supramolecular Materials*, MCIN/AEI (Research Network RED2018-102331-T), Nov. 2019 - Dec. 2021, **IP**: A. Frontera, 14 Partners, J. Aragó (GL) E. Ortí (researcher).
4. *Disruptive Organic Materials for Photovoltaics*, MCIN/AEI (Research Network RED2018-102815-T), Nov. 2019 - Dec. 2021, **IP**: N. Martín, 15 Partners, E. Ortí (group leader).
5. *Chemical Modification of Graphene*, MINECO (CTQ2015-71936), Dec. 2015 - July 2018, **IP**: F. Langa, 10 Partners, E. Ortí (group leader).
6. Organizer/coorganizer of 4 national conferences/schools and 1 international, 18 international scientific workshops and 11 divulgative open-doors meetings.