MINISTERIO DE CIENCIA E INNOVACIÓN

Cofinanciado por la Unión Europea

AGENCIA ESTATAL DE INVESTIGACIÓN

CURRICULUM VITAE ABREVIADO (CVA)

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

CVA date	11-3-2025

Part A. PERSONAL INFORMATION

First name	Juan Carlos		
Family name	Otero Fernández de Molina		
Gender (*)	Male	Birth date	
ID number			
e-mail		URL Web https://www.uma.es/departamento-quimica-fisica/info/105144/grupo-fqm103/	
Open Researcher and Contributor ID (ORCID) (*)		0000-0003-4078-6258	

(*) Mandatory

A.1. Current position

Position	Full Professor			
Initial date	03-08-2002			
Institution	Universidad de Málaga			
Department/Center	Química Física	Facultad de Ciencias		
Country	Spain		Teleph. number	
Key words	Raman, SERS, Molecular Structure, Nanoscience, charge transfer			

A.2. Previous positions (research activity interuptions, indicate total months)

Period	Position/Institution/Country/Interruption cause
1/10/1981-4/1/1984	Profesor Ayudante/Universidad de Extremadura
5/1/1984-20/11/1987	MEC Fellow/Universidad de Málaga
21/11/1987-10/10/1988	Profesor Titular de Universidad/Universidad de Granada
11/10/1988-2/8/2002	Profesor Titular de Universidad/Universidad de Málaga
3/8/2002-	Catedrático de Universidad/Universidad de Málaga

A.3. Education

PhD, Licensed, Graduate	University	Year
Lic. en Ciencias Químicas	Extremadura	1981
Doctor en Química	Málaga	1986

(Include all the necessary rows)

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

My career has been developed in three universities, University of Extremadura, as Assistant Professor (1981-1984), University of Malaga (1984-1987), as predoctoral fellow of MEC, and I have been Profesor Titular at the Universities of Granada (1987-1988) and Málaga (1988-2002) where I obtained the position of Catedrático de Universidad (2002-). I have recognized 6 teaching and research periods and the 5 periods of the regional administration.
My research is mainly of fundamental character in the fields of spectroscopy and molecular structure, having spent pre and postdoctoral stays at the Universities of Coimbra and Florence. I am coauthor of 165 JCR articles and have participated in projects financed both by the Spanish Ministry from 1982 to 2019 (since 2009 as PI) as well as in regional excellence projects since the first call. I have been PI of one of the 22 projects funded in the only call of the Spanish Strategic Action on Nanoscience and Nanotechnology (NAN2004-09312-C03).
In the last years I have been especially dedicated to the study of SERS (Surface-Enhanced Raman Scattering), where we have made relevant contributions on the origin of the

phenomenon, that is, on the mechanisms involved in the enormous intensification of the Raman signal of molecules in the presence of nanometric metal aggregates.
This issue has been controversial since the SERS discovery and has limited its development for forty years due to the complexity of the phenomenon where interfaces with systems of different size (nano/macroscopic metals and molecules) are involved as well as the surface excess of charge, electric fields and photon excitation.
My interest is to develop a methodology for analyzing SERS able of predicting the effect of different mechanisms on a particular spectrum. We are developing a novel methodology to simulate the effect of the electrical potential of the interface, i.e., of the excess of charge of the metal, in SERS. Until the last project, the study has been focused on metal-molecule photoinduced charge transfer (CT) processes. Faced with simplistic views based on Coulomb interactions, our results indicate that the metal charge is a determining factor in the electronic structure of the system, which tunes the energy to the metal-molecule CT states in an unexpected way as well as of the states located inside the metal or in the adsorbate itself.
Some of the most striking results have been to be able to explain the huge gain observed in the conversion between applied electrical potentials and the displacements of CT states or the lack of equivalence between direct metal-to-molecule and reverse molecule-to-metal CT processes due to the existence of two kinds of surface complexes. These two types of complexes are totally different in nature and are selected at positive and negative excess of charge respectively.
These results can be useful in the areas of physics (molecular electronics, nanoplasmonics, photovoltaics, etc.), materials (molecular materials, optoelectronics, LED devices, etc.) or in other specialties of chemistry, such as adsorption, heterogeneous catalysis or electrochemistry with or without photonic excitation. In all these fields, the complex and very little-known electronic structure of charged metal-molecule hybrids controls the structure and all their properties, so that the SERS can become a very powerful technique for get insight into charged hybrid systems with a molecular detail.
We collaborate with other research groups from the Universities of Coimbra (Luis A. Batista and Paula Marques, Raman spectroscopy in molecular biology), Paris-Saclay (Daniel Peláez Ruiz, molecular structure and dynamics) and with groups of the Italian CNR (Fabrizio Santoro, in Pisa, calculations of electronic structure and electronic spectroscopy) and CSIC (Santiago Sánchez Cortés, SERS and nanoplasmonics). A new collaboration has been established very recently with Mijeong Kang (Pusan National University, Busan) and Dong-Ho Kim (Korea Institute of Materials Science, Changwon) based on supramolecular chemistry for ultrasensitive performance of SERS, studying the effect of intercalating agents in metal-molecule charge transfer processes.
I have been chairman of the Spanish Spectroscopy Group of SEDOPTICA and member of the European Committee on the Spectroscopy of Biological Molecules (ECSBM) what allows me to have chaired/participated in the organizing commitees of national, Iberian, European and international spectroscopy meetings, giving invited talks on the subject of the project in several conferences listed below.
In addition, I have been part of the Committee of Experts for the evaluation of projects of the National R+D+I Plan (2004-2007) and I am reviewer of the AEI and ACSUCYL, ACPUA and other regional Spanish and foreign (Argentina, Portugal, Chile, Poland) agencies.

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

C.1. Publications *(see instructions)*
Ten selected publications in the last five years related to the project:

- M. Lemos de Sousa, S. Valdivia, J.C. Otero, I. López-Tocón (**2023**). Sensing Bisphenol A by Means of Surface-Enhanced Raman Spectroscopy and DFT Calculations to Elucidate the Enhancement Mechanism That Dominates the Spectrum, *Chemosensors* **11**, 78.
- D. Aranda, F. García-González, F. Avila, I. López-Tocón, J. Soto, J.C. Otero **(2022).** Computational Model for Electrochemical Surface-Enhanced Raman Scattering: Key Role of the Surface Charges and Synergy between Electromagnetic and Charge-Transfer Enhancement Mechanisms, *J. Chem. Theory Comput.* **18**, 6802–6815.

- S. Valdivia, F.J. Avila Ferrer, J.C. Otero, I. López-Tocón (**2022**). Voltage selection of physisorbed or chemisorbed 4-cyanobenzoate on a nanostructured silver electrode and the dual electronic structure of charged metal-molecule hybrids, *Appl. Surf. Sci.* **579**, 152071.
- I.B. Ansah, D. Aranda, H.S. Jung, S.-G. Park, M.Kang, J.C. Otero, D.-H. Kim (**2021**). Dual Synergistic Modulation of Photo-Induced Electron Transfer Processes Between Molecules and Gold Nanopillars for Ultrasensitive Plasmon-Enhanced Raman Scattering, *J. Mater. Chem. C*, **9**, 8842-8848.
- J. Soto, D. Peláez, J.C. Otero (**2021**). A SA-CASSCF and MS-CASPT2 study on the electronic structure of nitrosobenzene and its relation to its dissociation dynamics, *J. Chem. Phys.* **154**, 044307.
- S. Valdivia, D. Aranda, F.J. Avila Ferrer, J. Soto, I. López-Tocón, J.C. Otero (**2020**). Proving the dual electronic structure of charged metal-molecule interfaces: surface-enhanced Raman scattering of cyanide adsorbed on a nanostructured silver electrode. *J. Phys. Chem. C* **124**, 17632-17639.
- M. R. López-Ramírez, D. Aranda, I. López-Tocón, J. Soto, J. L. Castro, J.C. Otero **(2020).** Differentiated adsorption of thiobenzoic acid and thiobenzamide on silver nanoparticles determined by SERS spectroscopy *Spectrochim. Acta Part A* **246**, 119048.
- López-Tocón, S. Valdivia, J. Soto, J.C. Otero, F. Muniz-Miranda, M.C. Menziani, Maurizio Muniz-Miranda. **(2019)** A DFT Approach to the Surface-Enhanced Raman Scattering of 4-Cyanopyridine Adsorbed on Silver Nanoparticles. *Nanomaterials*, **10**, 2339.
- D. Aranda, S. Valdivia, J. Soto, I. López-Tocón, F.J. Avila, J.C. Otero. **(2019)** Theoretical Approaches for Modeling the Effect of the Electrode Potential in the SERS Vibrational Wavenumbers of Pyridine Adsorbed on a Charged Silver Surface. *Front. in Chem.* **7**, 423.
- D. Aranda, S. Valdivia, F.J. Avila, J. Soto, J.C. Otero, I. López-Tocón. **(2018)** Charge transfer at the nanoscale and the role of the out-of-plane vibrations in the selection rules of surface-enhanced Raman scattering. *Phys. Chem. Chem. Phys.,* **20**, 29430-29439.

C.2. Congress, indicating the modality of their participation (invited conference, oral presentation, poster)
Ten invited talks related to the project given by the IP:

- AAAFM-UCLA-2021 (American Association for Advances in Functional Materials) Los Angeles (US) 2021.
- VIII ICOPVS (8th International Conference on Perspectives in Vibrational Spectroscopy) Bangalore (India) 2020.
- ICAVS-10 (10th International Conference on advanced Vibrational Spectroscopy) Auckland (New Zealand) 2019.
- SERS-Xiamen, Xiamen (China) 2017.
- XXXVI-Reunión Bienal de la RSEQ, Sitges (Spain) 2017.
- ICAVS-9 (International Conference on advanced Vibrational Spectroscopy), Victoria (Canada) 2017.
- CCCE2016 (99th Canadian Chemistry Conference and Exhibition) Halifax (Canada) 2016.
- XXXV CSI (35th Colloquium Spectroscopicum Internationale) Xiamen (China) 2007.
- SRS2000 (1st International Symposium on Progress in Surface Raman Spectroscopy: Theory, Techniques and Applications) Xiamen (China) 2000.
- XVI ICORS (16th International Conference on Raman Spectroscopy), Cape Town (South Africa) 1998.

C.3. Research projects, indicating your personal contribution. In the case of young researchers, indicate lines of research for which they have been responsible.

Projects in which I have participated as IP whose development has been carried out, in whole or in part, during the last five years:

Research Projects:

Project name: Espectroscopía y estructura electrónica de interfases cargadas metal-molécula
PIs: Juan Carlos Otero, Isabel López Tocón
Program: Junta de Andalucía FEDER 2014-2020 (UMA18-FEDERJA-049)
Start: 01/10/2019 Funding amount: 40.115,26
Project name: Anticancer activity of novel polyamine Pd(II) complexes. A multidisciplinary study
PI / PI (Spanish partner): M. Paula M. Marques / Juan Carlos Otero
Program: Ministério da Ciência e Tecnologia (Portugal) (PTDC/QUI/66701/2006)
Start: 01/01/2019 Funding amount: 149.989
Project name: Procesos Energéticos en Híbridos Cargados metal-molécula
PI: Juan Carlos Otero Fernandez de Molina
Program: Plan Nacional de I+D (CTQ2015-65816-R)
Start: 01/01/2016. Funding amount: 93.170
Project name: Molecular cancer diagnostics by vibrational spectroscopy
PI / PI (Spanish partner): Luis Aberto Batista / Juan Carlos Otero
Program: FCT- Ministério da Educação e Ciência, Portugal (C491215625-00083205)
Start: 01/01/2018. Funding amount: 239.940

Scientific Equipment Projects:

Project name: Ampliación de la Unidad de Espectroscopía y Microscopía No Lineal de los Servicios Centrales de Apoyo a la Investigación
PI: Juan Carlos Otero
Program: Junta de Andalucía, Ayudas a Infraestructuras y Equipamientos I+D+I (EI19_092 UMA) Start: 23/06/2020 Funding amount: 188.089
Project name: Láser con emisión dual de pulsos de femtosegundos para potenciar la Unidad de Espectroscopía y Microscopía No Lineal del SCAI en aplicaciones multifotónicas no lineales y resueltas en el tiempo
PI: Juan Carlos Otero
Program: Ministerio de Ciencia, Innovación y Universidades, Infraestructuras Científicas (EQC2018-004504-PQ2918001E) Start: 01/01/2019 Funding amount: 301.296

Projects in which I have participated as researcher during the last five years:

Research Projects:

Project name: Materiales Nanoestructurados y/o funcionalizados para aplicaciones químicas
PI del consorcio: Tomás Cordero Alcántara (Ingeniería Química).
Program: Junta de Andalucía PAIDI (P18-RT-4592)
Start: 01/11/2020 Funding amount: 103.000

C.4. Contracts, technological or transfer merits, Include patents and other industrial or intellectual property activities (contracts, licenses, agreements, etc.) in which you have collaborated. Indicate: a) the order of signature of authors; b) reference; c) title; d) priority countries; e) date; f) Entity and companies that exploit the patent or similar information, if any

I have been IP of 8 contracts with alimentary industries located at Málaga devoted to the chemical analysis of their products (refs. UMA: 8.06/540.4602, 8.06/540.4603, 8.06/540.4604, 8.06/540.4605, 8.06/540.4606, 8.06/5.40.5103, 8.06/5.40. 5739, 8.06/5.40.5746) amounting to 39.650 €.