MINISTERIO DE CIENCIA E INNOVACIÓN

Cofinanciado por la Unión Europea

AGENCIA ESTATAL DE INVESTIGACIÓN

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	Sep 2022

First name	Ángel		
Family name	Martín Pendás		
Gender (*)	Male	Birth date (dd/mm/yyyy)	04/04/1965
Social Security, Passport, ID number	DNI 50064283E		
e-mail	ampendas@uniovi.es	URL Webs: qtcovi.grupos.uniovi.es Google Scholar & ResearchGate pages available	
Open Researcher and Contributor ID (ORCID) (*)		0000-0002-4471-4000	

(*) Mandatory

A.1. Current position

Position	Full Professor in Physical Chemistry			
Initial date	31-01-2011			
Institution	Universidad de Oviedo			
Department/Center	Fac. Química	Dpto. Química Física y Analítica		
Country	Spain		Teleph. number	985103037
Key words	Theoretical and Computational Chemistry, Simulation of materials. Chemical Bonding. Quantum Chemical Topology.			

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

Period	Position/Institution/Country/Interruption cause
1996-2011	Prof. Titular Univ. /Universidad de Oviedo/ Spain /-
1993-1996	Prof. Titular Escuela Univ. /Universidad de Oviedo/ Spain/-
1989-1993	Prof. Asociado /Universidad de Oviedo/ Spain/-

A.3. Education

PhD, Licensed, Graduate	University/Country	Year
Bachelor in Chemistry	Oviedo	1988
Ph.D. in Chemistry	Oviedo	1992

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

Permanent professor at the University of Oviedo since 1992. My research profile focuses on *methodological* developments in theoretical and computational chemistry (TCC), particularly regarding fundamental aspects in the theory of chemical bonding in real space. Our research group in Oviedo is considered one of the pillars in the development of new ideas in quantum chemical topology (QCT). My strengths come from good methodological skills together with coding abilities. I have the conviction that the theory of chemical bonding has to be reformulated in terms of orbital invariant quantities, independent of the underlying

computational method used to obtain them. In the last 10 years we have worked in major extensions of QCT that are now mainstream and well cited. In the first one, we proposed a theory of interacting quantum atoms (IQA) that provides an exact partition of the molecular energy into ionic and covalent interactions. A cornerstone of this theory is the quantitative identification of covalent energies with exchange-correlation contributions. In this way, ambiguous chemical concepts acquire a physically sound foundation. As a consequence of these new ideas, we have shown that the bond critical points of QCT stem from covalent terms. We have also developed a full revision of the theory of the chemical bond in terms of the statistics of the distributions of electrons (EDF). Chemical bonds in this formulation appear as the result of the statistical dependence between the electron populations of two or more spatial regions (two- or multi-center bonding). The ideas and models developed in our group are intended to generate new knowledge at the core of chemistry, and thus we expect them to be long-ranged in time. The number of groups across the world that are using our IQA or EDF methods increases every year. In the long run, our aim is the unification of QCT/IQA/EDF in a self-contained interpretation of the chemical bond that might be easily incorporated to the standard electronic structure codes. This implies increasing the computational efficiency of our proprietary codes, together with invading new fields, like those of biological systems or the nature of the chemical bond in excited states, in which our voice is slowly being heard. Since 2007 I am the PI of the QTCOVI group. Since 2011, I have obtained funds in public exceeding 1M€, only for theoretical purposes. To this quantity we should add around 6M€ from projects in which I have participated. I maintain many international collaborations, e.g those with P. Popelier (Manchester), C. Gatti (Milán), J. Hernández-Trujillo, T. Rocha and R. Hernández-Lamoneda (México), A. Savin, J. Contreras, B. Braïda (UPMC, París), E. Espinosa (U. Lorraine), M. Kohout and K. Finzel (Max Planck Institute), F. Muñoz and C. Cárdenas (Chile), etc. I have supervised graduate, postgraduate, doctoral, and postdoctoral students, around 15 in the last 10 years. All the postdoctoral students under my supervision hold international academic positions (Mexico, Ireland). Several of my Ph. D students hold permanent positions at the Spanish academia, and most of the rest are enjoying postdoctoral stays, or have found their place in the private sector. Since 2011, our projects have obtained 3 FPI PhD students in a row. Almost all the remaining PhD students obtained their grants in competitive (FPU, regional) calls. I am an active member of the theoretical chemistry community, having organized two international conferences in Oviedo (ESPA2010, ESCB2-2018), and having been the main editor of article collections in TCC peer-reviewed journals. Since our methodological work is not close to technological transfer, I have devoted efforts to disseminate it to the society, participating in the European researchers' night and other similar initiatives. I am finishing (with Dr. Julia Contreras) a textbook on topological approaches to chemical bonding that will be published by Springer in 2022. We expect it to be part of future graduate textbooks in chemistry. I actively participate in the evaluation of scientific research, having been an ANECA panelist in chemical physics, and evaluating projects continuously over the years for ANECA, BSC, the Galician, Andalusian and Aragon scientific agencies, and international ones like the NSF (USA), CONACYT (Mexico), CONICYT (Chile), FWO (Belgium), BPI (France), or their Polish and South African analogs, among others. I was elected in 2019 as president of the European Committee for Chemical Bonding (ECCB), a non-profit society that pursues the development of the theory of the chemical bond. I am associate editor of the journal *Molecules* since 2019 and member elect of the WATOC board since July 2022. A summary of my scientific production: 240+ indexed papers/book chapters. 50+ invited/plenary talks. *h*/number citations: 49, 10k citations I have supervised 8 + (2 in progress) Ph.D. Theses. I am in the world top two percent scientists Stanford list.

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

C.1. Publications ***(*****10 relevant pubs. since 2010)**

1. A. Martín Pendás*, E. Francisco, *"The role of references and the elusive nature of the chemical bond". Nat. Commun.* 10.1038/s41467-022-31036-6 (2022)

2. A. Gallo-Bueno, M. Kohout, E. Francisco, and A. Martín Pendás*, "*Localization and Delocalization in Solids from Electron Distribution Functions", J. Chem. Theory Comput.* 10.1021/acs.jctc.2c00234, 2022.
3. S. Sowlati-Hashjin1, V. Vojtěch Šadek2,3, S. SeyedAbdolreza Sadjadi4, M. Mikko Karttunen A.Martín Pendás, C.Foroutan-Nejad., "*Collective interactions among organometallics are exotic bonds hidden on lab shelves". Nat. Commun*, 10.1038/s41467-022-29504-0 (2022)
4. G. Acke, S. De Baerdemacker, A. Martín Pendás*, P. Bultinck*, "*Hierarchies of quantum chemical descriptors induced by statistical analyses of domain occupation number operators". WIREs Comp. Mol. Sci*. 2020, DOI: 10.1002/wcms.145 (2019)
5. S. Gil, A. Peña, N. Ramos-Berdullas, A. Martín Pendás*, M. Mandado*. "*Assessing the Reversed Exponential Decay of the Electrical Conductance in Molecular Wires: The Undeniable Effect of Static Electron Correlation". Nano Letters*, **19**, 7394-7399, 2019.
6. C. Outeiral, M. A. Vincent, Á. Martín Pendás*, P. L. A. Popelier*, "*Revitalizing the concept of bond order through delocalization measures in real space". Chem. Sci.* **9**, 5517-5529, 2018.
7. E. Romero-Montalvo, J. M. Guevara-Vela, W. Vallejo, A. Costales, A. Martín Pendás, M. Hernández Rodríguez, T. Rocha-Rinza*, "*Bifunctional catalytic role of water clusters in the formation of acid rain". Chem. Commun.* **53**, 3516-3519, 2017.
8. A. Gallo-Bueno, M. Kohout, A. Martín Pendás*, 2016, "*Decay Rate of Correlated Real-Space Delocalization Measures: Insights into Chemical Bonding and Mott Transitions from Hydrogen Chains". J. Chem. Theory. Comput*. **12**, 3053-3062, 2016.
9. P. Maxwell, A. Martín Pendás, P. L. A. Popelier*, "*Extension of the interacting quantum atoms (IQA) approach to B3LYP level density functional theory (DFT)". Phys. Chem. Chem. Phys*. **18**, 20986-21000, 2016.
10. J. M. Guevara-Vela, R. Chavez-Calvillo, M. Garcia-Revilla, J. Hernandez-Trujillo, O. Christiansen, E. Francisco, A. Martín Pendás*, "*Hydrogen-Bond Cooperative Effects in Small Cyclic Water Clusters as Revealed by the Interacting Quantum Atoms Approach". Chem. Eur. J*. **19**, 14304-14315, 2013.

C.2. Congress (10 relevant contributions in the last 10 years. Authors, Title, Conference, Invited/Plenary)

When several authors participated, the presenting one is underlined.

1. Ángel. Martín Pendás. *Interacting Quantum Atoms*: *Meeting Chemical Intuition from a Real Space Perspective*. 10th TCCW Conference. Tehran (Iran, Online). 23-25 November 2021. Plenary.
2. Ángel. Martín Pendás. *Counting electrons in atoms (within molecules). New models, new insights?* Chemical Concepts and Quantum Chemistry 2019. 18-20 November. Heidelberg (Alemania). Invited.
3. Ángel Martín Pendás. *Real space regions as open quantums systems*. Blas Cabrera Physics Seminar. La Laguna (España). 3-4 September 2019. Plenary.
4. Ángel Martín Pendás, *Should charge-shift bonding be reconsidered?* CTTC 2019. Quito (Ecuador). 1-5 July. Invited.
5. Ángel Martín Pendás. *The Quantum Theory of Atoms in Molecules and the AIMAll software*. TCB Workshop. Bremen (Germany) 2019. 14-19 July. Plenary.
6. Ángel Martín Pendás. *Quantum Chemical Topology as a theory of open quantum systems*. CCTC18. Changsha (China) 2018, 7-12 December 2018. Invited.
7. Ángel Martín Pendás. *Intrinsic Bond Energies: A real space point of view.* Theoretical Chemistry Colloquium. Marburg, (Alemania) Jan 10th, 2017. Plenary.
8. Ángel Martín Pendás, E. Francisco. *One electron images in real space: natural adaptive orbitals*. International Conference on Chemical Bonding. Kawaii (hawaii) 22-26 June 2017. Invited.
9. Ángel Martín Pendás. *Chemical bonding in real (or position) space: Interacting Quantum Atoms*. Uspex11 conference, 5-9 June 2016, Villa Monastero, Varenna, Lake Como, Italy. Plenary.

10. Ángel Martín Pendás, E. Francisco. *Chemical bonding theory from electron distribution functions*. The Chemical bonds at the 21st Century. Xiamen (China) 14-19 June 2015. Invited.

C.3. Recent Relevant Research projects (Reference, Title, Funding Agency, Call, Duration, Role, Amount, Granted/Pending)

1. Reference: **PID2021-122763NB-I00**. Title: *Topología Químico Cuántica y su tretroalimentación con el aprendizaje automático, la teoría del enlace químico y la catálisis.* Funding agency: MICINN, Plan nacional, Investigación de excelencia, Call 2021. Duration, from: September 2022 to september 2025. Principal Investigator: Ángel Martín Pendás. Amount: 120.000 €**.** Granted.
2. Reference: **IDI-2021-000054**. Title: *Química Teórica y Computacional*. Funding agency: Ficyt. Convocatoria ayuda a grupos consolidados 2014, 2017. Duration, from: January 2022 to 2025. Principal Investigator: J. Manuel Recio. Amount: 86.000 €. Granted (Provisional resolution).
3. Reference: **PGC2018-095953-B-I00**. Title: *Topología Químico Cuántica como una ciencia aplicada: de la teoría a la modelización biomolecular y los materiales avanzados*. Funding agency: MICINN, Plan nacional, Investigación de excelencia, Call 2018. Duration, from: January 2016 to 2018. Principal Investigator: Ángel Martín Pendás. Amount: 145.200 €**.** Granted.
4. Reference: **CTQ2015-65790-P**. Title: *Progreso En Topología Químico Cuántica Cuantitativa: De La Estadística De Poblaciones Electrónicas A La Modelización Biomolecular* Funding agency: Mineco, VI Plan nacional, Investigación de excelencia, Call. 2015. Duration, from: January 2016 to 2018. Principal Investigator: Ángel Martín Pendás. Amount: 104.302 €**.** Granted.
5/6. Reference: **Grupin14-049/ IDI-2018-000177**. Title: *Química Teórica y Computacional*. Funding agency: Ficyt. Convocatoria ayuda a grupos consolidados 2014, 2017. Duration, from: January 2015 to 2017, 2018 to 2021. Principal Investigator: Ángel Martín Pendás. Amounts: 165.000/164.000 €. Granted.
7. Reference: **CTQ2012-31174/BQU**. Title: *Estadística De La Distribución Electrónica en el Espacio Real: Relevancia para la Teoría del Enlace Químico en moléculas y cristales*. Funding agency: Mineco, VI Plan nacional, Investigación no orientada, Call. 2012 Duration, from: January 2013 to 2015. Principal Investigator: Ángel Martín Pendás. Amount: 102.960 €. Granted.
8. Reference: **CTQ2009-08376/BQU**. Title: *Avances en Topología Químico Cuántica.* Funding agency: MICINN. Plan Nacional, Investigación No orientada. Duration, from: January 2010 to 2012. Principal Investigator: Ángel Martín Pendás. Amount: 79.860 €. Granted.
9. Reference**: CSD2007-00045**. Title: *MALTA (Materia a alta presión).* Funding agency: MEC Programa Consolider-Ingenio 2010. Duration, from: January 2007 to 2012. Principal Investigator: Valentín García Baonza. Role: Researcher. Amount: 5.000.000 €. Granted.

C.4. Contracts, technological or transfer merits

Given the methodological nature of our research, we have no contracts or patents. We do write computational codes that are made accessible to the international community. Since 2011 we have released CRITIC (versions 1,2), EDF (versions 1,2) all published in *Comput. Phys. Commun*. and PROMOLDEN (unpublished). All freely available.