SHORT CURRICULUM VITAE OF OCTAVIO RONCERO

Part A. Personal Data

Date	27/04/2018

Name	Octavio Roncero Villa		
Identity card	02525074L	Age	56
Research ID's	Researcher ID	K-1872-2014	
	Código Orcid	0000-0002-8871-4846	

A.1. Situación profesional actual

Institution	Consejo Superior de Investigaciones Científicas			
Department	Instituto de Física Fundamental			
Address	Serrano, 123			
Phone	915616800	e-mail	Octavio.roncero@csic.es	
Position	Investigador científico		Starting date	2002
UNESCO codes	2206 – 2207 - 2208			
Keywords	Molecular Physics, Chemical Physics, Astrochemistry			

A.2. Academic training

title	University	Year
Master in Chemistry	Autónoma de Madrid	1984
PhD in sciences	Autónoma de Madrid	1987

A.3. General Indicators of the scientific production

- 4 PhD students supervised, 1 PhD supervision in progress, 3 master student supervised
- Citations: 3604 (Web of Science) - 4264 (Google Scholar).
- H index= 33. (Web of Science) - 36 (Google Scholar)
- 65 invited conferences in international congress
- 145 publications in Scientific journals

Parte B. Brief summary of the scientific activity

Theoretical study of dynamical processes in molecular systems, such as photodissociation, colissions and spectroscopy, with emphasis in the development of methods and codes to simulate different measured quantities in different kind of experiments. I want to stress the paper **J. Compt. Phys. 94 (1991) 59,** presenting a comparative study of different quantum methods for the propagation of wave packets, with more than 740 references, has become a classic in the field.

I started with the study of photodissociation processes, developing time independent close coupling methods and codes. In the reference J. Chem. Phys. 92 (1990) 3348 (95 citations) I studied the predissociation of van der Waals complexes with one of the first three-dimensional calculation at that time. In J. Chem. Phys. 100 (1994) 3610 (159 citations) I did the first fully quantum treatment of the correlation among the polarization of products, the polarization of light and the angular distribution products in direct photodissociations.

Later I studied reactive collisions and transition state spectroscopy processes, developing codes and methods for the quantum propagation of wave packets. In J. Chem Phys. 107 (1997) 10085 (83 citations), I did one of the first exact quantum calculations using time dependent methods for a triatomic system with three different atoms. In J.Chem.Phys. 125 (2006) 054102 (90 citations), I developed a method to calculate the state-to-state reaction cross sections og reactive collisions using quantum wave packet methods. In J.Phys. Chem A. 113(2009)14488 (58 citations) I developed a highly parallelized code for quantum wave packet propagation which allowed the full quantum study of the correlation between the relative velocity vectors of reactants and products and their rotational polarization.

I have developed methods for the analytical representation of potential energy surfaces (PES), acquiring experience in highly correlated electronic ab initio methods and calculations. In J. Chem. Phys. 112 (2000) 1240 (85 cites) we developed a PES of spectroscopic accuracy for H_3^+. In J. Chem. Phys. 133 (2010) 024306 (44 cites), we developed a global PES in 9 dimensions for H_5^+ with a new method called "triatomics-in-molecules". Later, we applied it to the H_4^+ system, and recently we have extended the method to even larger systems such as H2CO+OH (in ApJ 850 (2017) 28) and to CH3OH +H (in progress) to study the reactivity of organic molecules at low temperatures (T< 100K).

I have studied the reactivity on metallic nano-structures and clusters using DFT methods. In J. Chem. Phys. 129 (2008) 184104 (57 citations), I developed a method for the obtaining of embedding potentials, based on the partition of the total electronic density, for the use of highly correlated methods in one of the subsystems. In PCCP 11 (2009) 10122 (21 citations) we studied the dissociation of H_2 in gold nano-structures. This has been extended to study the relationship between the H_2 dissociation and the electronic conduction through a gold nanowire (Phys.Rev.B, 90, 041404 (R) (2014)).

Nowadays I am working in some coordinated projects, national (such as a CONSOLIDER project ended in 2017) and European (one COST and one Synergy-ERC) astrophysics groups with the aim of calculating rates for several reactions, specifically of COMSs between 10K and 100K and subject of the current proposal, in order to introduce them in models to check the physical conditions of the different astrophysical environments

C.1. 5 Selected publications of the last 10 years

1. "Differential cross sections and product rotational polarization in A+BC reactions using wave packet methods: $H^+ + H_2$ and Li + HF examples", A. Zanchet, **O. Roncero**, T. González-Lezana, A. Rodríguez-López, A. Aguado, C. Sanz.Sanz y S. Gómez-Carrasco, J. Phys. Chem. A, **113** (2009) 14488 **(58 citations).**
   In this work we have developed a fully parallelized code for the study of quantum wave packet state-to-state cross sections of chemical reactions, the MADWAVE3 open source code. This code is currently used by several groups and allows the calculation of differential cross section of triatomic systems and study the effect of the rotational polarization of reactants and products.

2. "An inversion technique for the calculation of embedding potentials", **O. Roncero**, M.P. de Lara-Castells, P. Villarreal, F. Flores, J. Ortega, M. Paniagua y A. Aguado, J. Chem. Phys. 129 (2008) 184104 **(57 citas).**
   Development of a method to obtain embedding potentials to calculate electronic properties using highly correlated methods in one of the subsystems. This method is based on a partition of the electronic density of the whole system in several densities of the subsystems, such as each of densities of the subsystems is the solution of a modified Fock equation, including an embedding potential, optimized to this aim. This work have originated to a series of methods developed by several groups in order to improve the force fields normally used in QM/MM methods and to study the electronic spectroscopy of chromophores in a larger environment.

3. "A new accurate and full dimensional potential energy surface of H_5+ based on a triatomics-in-molecules analytical form", A. Aguado, P. Barragán, R. Prosmiti, G. Delgado-Barrio, P. Villarreal y **O. Roncero**, J. Chem. Phys. **133** (2010) 024306 **(44 citations).**
   We have developed an analytic description of the potential energy surface including all 9 dimensions of the H5+ system. This PES is based on highly accurate ab initio points and describe all rearrangements exchange channels of $H_2 + H_3^+$ including the long-range interaction with high accuracy and being invariant under any permutation of the atoms. These properties are required to accurately describe the exchange reactions at low temperatures important in the deuteration processes and the ortho/para conversion process of H_3^+. This surface is based on a new method, called "triatomics-in-molecules", which allows the accurate description of two and three atomic fragments, adding a 5-body term in improve the accuracy in the short-interaction region.

4. "Dynamically biased statistical model for the ortho/para conversion in the $H_2+H_3^+ \rightarrow H_3^+ + H_2$ reaction", S. Gómez-Carrasco, L. González-Sánchez, A. Aguado, C. Sanz-Sanz, A. Zanchet y **O. Roncero**, J. Chem. Phys. **137** (2012) 09303, **(14 citations).**
   Development of a statistical model for the exchange reaction $H_2+H_3^+ \rightarrow H_3^+ + H_2$ and the ortho/para conversion of the two molecules of high astrophysical interest. To this aim, the nuclear spin is included and the full dimension potential is used, in contrast to previous studies that only use the asymptotic long-range interaction. In addition, a dynamical bias is introduced to mimic the competition between a direct hop and an indirect exchange mechanisms by using quasi-classical trajectories, correcting the zero-point energy using RRKM arguments. With this method the experimental hop/exchange ratio is reproduced in a semiquantitative way, finding that there is a transition between a statistical mechanism (at low temperatures below 100K) and a direct mechanism at higher temperatures.

5. "$H_2(v=0,1) + C^+(^2P) \rightarrow H + CH^+$ state-to-state rate constants for chemical pumping models in astrophysical media", A. Zanchet, B. Godard, N. Bulut, **O. Roncero**, P. Halvick, J. Chernicharo, AstroPhys. J, **766**, 80 (2013)", **(31 citations)**.
   In this work we propose the in diffuse clouds, characterized by relatively high temperatures, the CH^+ formation is due to the presence of vibrationally excited H_2. For this aim quantum state-to-state rate constants have being calculated and included in PDR astrophysical models, finding that the detected emission from highly rotational CH^+ fragments increase significantly when considering this chemical pumping model, in agreement with the observations.

C.2. Selected Scientific Grants in the last 10 years

1. RRHH member of the ERC project: "Gas and Dust from stars to the laboratory: exploring the NanoCosmos"
   Reference: Synergy project (I-ERC/2050)
   Funding agency: ERC
   Coordinator: José Cernicharo
   Period: 2014-2020
   Budget of RRHH member: 103538,45 euros

2. MC of COST Action CM-1401 'Our Astrochemical History". Period: 2014-2018 Spanish MC , Co-lider WG4 "isotopic Chemistry until January 2017, Lider WG1 "Gas phase chemistry" from January 2017

3. "Quantum simulation of state-to-state rate constants for the formation of hydrides in reactive collisions and their radiative constants for chemical pumping models in astrophysical media"
   Reference: I-LINK0775
   Funding Agency: CSIC.
   Budget: 14.800 €
   Period: 2010-2015 (extensión hasta diciembre 2016)
   Principal Researcher: Octavio Roncero Villa

4. "Molecular Astrophysics". Programa: Consolider – Ingenio 2010
   Reference: CSD2009-00038
   Funding Agency: Ministerio de Ciencia e Innovación
   Period: 2010-2017
   Coordinator: José Cernicharo Quintanilla
   Principal researcher of ABIDIN-CSIC group: Octavio Roncero
   Budget of ABIDIN-CSIC group: 101.000 euros

5. "NanoObjects: from atoms to viruses"
   Reference: S-2009/MAT-1467
   Funding Agency: Comunidad Autónoma de Madrid
   Period: 2010 - 2014
   Coordinator: Julio Gómez Herrero (UAM)
   Principal researcher of IFF-CSIC group: Octavio Roncero
   Budget IFF-CSIC group: 30.000 €

6. "Propiedades Mecánicas, eléctricas y catalíticas de nanoobjetos: síntesis, caracterización y modelización"
   Reference: S-0505/MAT/0303
   Funding Agency: Comunidad Autónoma de Madrid
   Period: 2006 - 2009
   Coordinator: Fernando Flores (UAM)
   IP of IFF-CSIC group: Octavio Roncero
   Budget: 43.500 €

7. "Procesos dinámicos y estocásticos en astrofísica molecular y en la interacción gas superficie"
   Funding Agency: Ministerio de Economía y competitividad
   Reference: FIS2014-52172-C2
   Period: 2015 – 2018
   IP's: Octavio Roncero Villa y Salvador Miret Artés
   Budget: 30.250€

C.3. Other

1. Master Course "Dinámica de reacciones químicas y femtoquímicas"
   Programa de doctorado interuniversitario "Química Física Aplicada", at Universidad Autónoma de Madrid and Universidad Complutense de Madrid.
   Years: 04/05, 05/06, 06/07 y 08/09.
2. Course entitled "Teoría cuántica de colisiones moleculares" (40 hours) in the Doctoral Master about "Simulación de procesos moleculares" of the Universidad Autónoma de Madrid.. Coordinator: Prof. M. Paniagua. Year: 06/07
3. Course (2 hours) entitled "Dynamique réactionnell et processus photoinitiés". School of "Dynamique réactionnelle" du Réseu Francaise de Chimie Théorique (RFCT) (UEPCT10), at Presqu'ile de Giens (Francia). Coordinator: Prof. Didier Lemoine. Date 2-7 de septiembre 2007
4. Course (2 hours) "Reaction dynamics". In the "Training school: the chemical Cosmos". Hold in Grenoble (France), March 18-22 2013.
5. Co-chairman of the "14th International Workshop on Quantum Systems in Chemistry and Physics" (QSCPXIV), hold in San Lorenzo de El Escorial, September 13-19th 2009.
6. Member of the Scientific organizing committee of the "2nd National conference on laboratory and molecular astrophysics", hold in Sevilla, November 2012.
7. Member of the Scientific organizing committee of the COST workshop "theory and modelling of polarization in astrophysics", hold in Prague (Czech Republic), Mayo 2-4th 2014.
8. Chairman of the workshop "Quantum Reactive Scattering" 2015, Salamanca, July 6-10th 2015, http://fama.iff.csic.es/con/QRS-2015/
9. Chairman of the Cost Workshop "Gas phase Cold chemistry of COMs: a challenge for experiments, theory and astrophysical modeling", hold in Ciudad Real (Spain), December 10-13 2017, http://fama.iff.csic.es/con/COMS2017/