



# Cristina Sanz Sanz

## Curriculum Vitae

Associate Professor  
Departament of Applied Physical Chemistry  
Autonoma University Madrid, Spain  
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### Education

- 2005 **European PhD**,  
Autonoma University Madrid  
Supervisors: Prof. Miguel Paniagua Caparrós (UAM), Dr. Octavio Roncero Villa (Institute of Fundamental Physics (IFF), CSIC)  
Title: *Probing ground and excited electronic states of LiHF and CaHCl systems to understand the harpoon mechanisms in collision and photoinitiated processes*
- 2002 **Diploma in Advanced Studies**,  
Autonoma University Madrid  
Supervisors: Dr. Alfredo Aguado (UAM), Dr. Octavio Roncero Villa (IFF, CSIC)  
Title: *Electronic structure calculations and quantum dynamics*
- 2000 **Degree dissertation**,  
Autonoma University Madrid  
Supervisors: Dr. Alfredo Aguado  
Title: *Potential energy surfaces of  $H_3^+$*
- 1998 **Bachelor degree in Chemistry**,  
Autonoma University Madrid  
*Speciality in Physical Chemistry*

### Academic/Scientific positions

- 2019- **Associate Professor**, UAM
- 2013-2018 **Assistant Professor**, UAM
- 2013 **Researcher**, Complutense University Madrid
- 2010-2013 **Researcher, CONSOLIDER project**, IFF, CSIC
- 2005-2006 **Interim Associate Professor**, UAM

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## Fellowships

- 2008-2010 **EPSRC Postdoctoral Fellowship**,  
Funded by the Engineering and Physical Sciences Research Council  
University of Birmingham, UK
- 2006-2008 **Postdoctoral Fellowship**,  
Funded by the Spanish Ministry of Education and Science  
University of Bristol, UK
- 2002-2005 **Postgraduate PhD fellowship I3P**,  
Funded by the Spanish National Research Council, IFF, CSIC
- 2001-2002 **Postgraduate fellowship THEONET**,  
Funded by the European project THEONET, University of Nijmegen, Netherlands
- 2001 **Postgraduate fellowship**,  
Funded by the Autonoma University Madrid, UAM
- 1999-2000 **Postgraduate fellowship CSIC**,  
Funded by the Spanish National Research Council, IFF-CSIC, Spain
- 1999 **FUAM internship**,  
Funded by the GESINAR company, GESINAR S.L.-UAM

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## Scientific projects (last 10 years)

- 2022-2025 **Interaction potentials of poliatomic systems - PID2021-122549NB-C22**, IPs: Dr. Cristina Sanz Sanz and Dr. Alfredo Aguado Gómez, Funded by Spanish Ministry of Science and Innovation
- 2018-2021 **Collisions and photodissociation of astrophysics interest in gas phase and ices and surface dynamics - FIS2017-83473-C2-2-P**, IP: Dr. Alfredo Aguado Gómez, Funded by Spanish Ministry of Science, Innovation and Universities
- 2015-2017 **Dynamics and stochastic processes in molecular astrophysics and in the gas-surface interaction - FIS2014-52172-C2-2-P**, IP: Dr. Alfredo Aguado Gómez, Funded by Spanish Ministry of Science, Innovation and Universities
- 2010-2015 **Molecular astrophysics: the Herschel and Alma era - CSD2009-00038**, IP: Dr. Octavio Roncero Villa, Funded by Spanish Ministry of Science and Innovation
- 2012-2014 **Structure, spectroscopy and dynamics of molecules and molecular clusters in interphases of gas/condensate mater in open systems - FIS2011-29596-C02-01**, IP: Dr. Octavio Roncero Villa, Funded by Spanish Ministry of Science and Innovation

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## Student supervision

### PhD supervision

- 2023- Mr Jorge Alonso de la Fuente.  
*Theoretical studies of Phosphine and its fragments.*  
Co-supervisor: Dr. Alexandre Zanchet (CSIC)
- 2022- Co-supervision of Mr Javier Hernández Rodríguez.  
*Dynamics of spin-forbidden mechanisms*  
Co-supervisor: Dr. Susana Gómez-Carrasco (USAL)

### Master projects supervision

- 2023 Co-supervisor of the master project of Mr Jorge Alonso de la Fuente.  
Title: *Phosphorous hydrides: where are they in the atmospheres of AGB stars?*.  
Co-supervisor: Dr. Alexandre Zanchet
- 2022 Co-supervisor of the master project of Mr Javier Hernández Rodríguez.  
Title: *Dynamics of spin-forbidden reactions*.  
Co-supervisor: Dra. Susana Gómez Carrasco
- 2020 Co-supervisor of the master project of Ms Cristina Ordás González.  
Title: *Study of the weak interactions of noble gases adsorbed in PAHs surfaces: comparison between canonical CCSD models and DLPNO variants*.  
Co-supervisor: Dr. Daniel Arismendi Arrieta
- 2019 Co-supervisor of the master project of Ms María Judit Montes de Oca.  
Title: *Computational spectroscopy of noble-gas complexes*.  
Co-supervisor: Dra. Rita Prosmi
- 2019 Co-supervisor of the master project of Ms Raquel Yanes Rodríguez.  
Title: *A quantum chemistry study of He-water inclusion compounds*.  
Co-supervisor: Dra. Rita Prosmi
- 2019 Co-supervisor of the master project of Mr Pablo Ortega Álvarez.  
Title: *Computational study of the cofactor-free oxygenation reaction in DpgC dioxygenase*.  
Co-supervisor: Dr. Pablo G. Jambrina
- 2019 Co-supervisor of the master project of Pablo Ramos Sánchez.  
Título: *Study of the absorption of wavepackets using non-static methods*.  
Co-supervisor: Dr. Manuel Lara Garrido

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### Publications (last 10 years)

1. J. Hernández-Rodríguez, C. Sanz-Sanz, P. Alberto Enríquez, M. González, and M. Paniagua. Potential energy surfaces for singlet and triplet states of the  $\text{LiH}_2^+$  system and quasi-classical trajectory cross sections for  $\text{H} + \text{LiH}^+$  and  $\text{H}^+ + \text{LiH}$ . *Phys. Chem. Chem. Phys.*, 25:28052, 2023.
2. L. González-Sánchez, E. Yurtsever, J. Alonso de la Fuente, C. Sanz-Sanz, R. Wester, and F. A. Gianturco. Collision-induced state-changing rate coefficients for cyanogen backbones  $\text{NCN } ^3\Sigma^-$  and  $\text{CNN } ^3\Sigma^-$  in astrophysical environments. *Phys. Chem. Chem. Phys.*, 25:30330, 2023.
3. J. Alonso de la Fuente, C. Sanz-Sanz, L. González-Sánchez, E. Yurtsever, R. Wester, and F. A. Gianturco. The  $\text{CH}^- ^3\Sigma^+$  anion: Inelastic rate coefficients from collisions with He at interstellar conditions. *J. Phys. Chem. A*, 127:765, 2023.
4. P. Ortega, S. Gil-Guerrero, L. González-Sánchez, C. Sanz-Sanz, and Pablo G. Jambrina. Spin-forbidden addition of molecular oxygen to stable enol intermediates. decarboxylation of 2-methyl-1-tetralone-2-carboxylic acid. *Int. J. Mol. Sci.*, 24:7424, 2023.
5. P. del Mazo-Sevillano, D. Félix-González, A. Aguado, C. Sanz-Sanz, D.-H. Kwon, and O. Roncero. Vibrational, non-adiabatic and isotopic effects in the dynamics of the

$\text{H}_2 + \text{H}_2^+ \rightarrow \text{H}_3^+ + \text{H}$  reaction: application to plasma modelling. *Mol. Phys.*, page e2183071, 1 2023.

6. J. Alonso De La Fuente, C. Sanz-Sanz, L. Gonzalez-Sanchez, E. Yurtsever, R. Wester, and F. A. Gianturco. The  $\text{CH}^-$  anion: Inelastic rate coefficients from collisions with He at interstellar conditions. *J. Phys. Chem. A*, 127:55, 1 2022.
7. J. Coonjobeeharry, K. E. Spinlove, C. Sanz-Sanz, M. Sapunar, N. Došlić, and G. A. Worth. Mixed-quantum-classical or fully-quantized dynamics? a unified code to compare methods. *Philos. Trans. Royal Soc. A*, 380, 2022.
8. C. Sanz-Sanz, A. Aguado, and O. Roncero. Near-resonant effects in the quantum dynamics of the  $\text{H} + \text{H}_2^+ \rightarrow \text{H}_2 + \text{H}^+$  charge transfer reaction and isotopic variants. *J. Chem. Phys.*, 154:104104, 3 2021.
9. P. Ortega, A. Zanchet, C. Sanz-Sanz, S. Gómez-Carrasco, L. González-Sánchez, and P. G. Jambrina. Dpgc-catalyzed peroxidation of 3,5-dihydroxyphenylacetyl-coA (DPA-CoA): Insights into the spin-forbidden transition and charge transfer mechanisms. *Chem. Eur. J.*, 27:1700–1712, 1 2021.
10. O. Roncero, V. Andrianarijaona, A. Aguado, and C. Sanz-Sanz. Vibrational effects in the quantum dynamics of the  $\text{H} + \text{D}_2^+$  charge transfer reaction. *Mol. Phys.*, page e1948125, 7 2021.
11. A. Aguado, O. Roncero, and C. Sanz-Sanz. Three states global fittings with improved long range: singlet and triplet states of  $\text{H}_3^+$ . *Phys. Chem. Chem. Phys.*, 23:7735–7747, 4 2021.
12. P. Ortega, S. Gil-Guerrero, A. Veselinova, A. Zanchet, L. González-Sánchez, P. G. Jambrina, and C. Sanz-Sanz. Multi- and single-reference methods for the analysis of multi-state peroxidation of enolates. *J. Chem. Phys.*, 154:144303, 4 2021.
13. C. Sanz-Sanz and G. A. Worth. Field modified spin-orbit potential curves of IBr. preliminary dynamical results. *Phys. Chem. Chem. Phys.*, 21:14429–14439, 7 2019.
14. N. Bulut, A. Aguado, C. Sanz-Sanz, and O. Roncero. Quantum effects on the  $\text{D} + \text{H}_3^+ \rightarrow \text{H}_2\text{D}^+ + \text{H}$  deuteration reaction and isotopic variants. *J. Phys. Chem. A*, 123:8766–8775, 10 2019.
15. C. Sanz-Sanz, A. Aguado, and O. Roncero. Non-adiabatic couplings and dynamics in proton transfer reactions of  $\text{H}_n^+$  systems: Application to  $\text{H}_2 + \text{H}_2^+ \rightarrow \text{H} + \text{H}_3^+$ . *J. Chem. Phys.*, 143:234303, 12 2015.
16. R. Manso Sainz, O. Roncero, C. Sanz-Sanz, A. Aguado, A. Asensio Ramos, and J. Trujillo Bueno. Depolarizing collisions with Hydrogen: neutral and singly ionized alkaline earths. *Astrophys. J.*, 788:118, 5 2014.

## Visits to academic institutions

- 2018 **University of Groningen, Netherlands**,  
 Research visit to the group of Dr. Shirin Faraji,  
 Duration: 3 days

- 2017 **Ruder Boskovic Institute Zagreb, Croacia,**  
Research visit to the group of Prof.<sup>a</sup> Nadja Džslíć,  
Duration: 10 days
- 2009 **National Research Council, Ottawa-Canada,**  
Research visit to the group of Prof. Albert Stolow,  
Duration: 1 week
- 2009 **Universidad de Alberta, Canada,**  
Research visit to the group of Prof. Albert Stolow,  
Duration: 3 semanas
- 2008-2010 **University of Birmingham, United Kingdom,**  
Postdoctoral research project in the group of Prof. Graham A. Worth,  
Duration: 2 years
- 2006-2008 **University of Bristol, United Kingdom,**  
Postdoctoral research project in the group of Prof. Gabriel G. Balint-Kurti,  
Duration: 2 años
- 2006 **CNRS, Laboratoire Francis Perrin, France,**  
Research visit to the group of Prof. Benoit Soep,  
Duration: 1 week
- 2005 **CNRS, Laboratoire Francis Perrin, France,**  
Research visit to the group of Prof. Benoit Soep,  
Duration: 3 months
- 2004 **University of Rome “La Sapienza”, Italy,**  
Research visit to the group of Prof. Francesco A. Gianturco,  
Duration: 1 month
- 2001-2022 **Radboud University Nijmegen, Netherlands,**  
Research visit to the group of Prof. Ad van der Avoird,  
Duration: 1 year

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## Courses in scientific schools

- 2022 **School on High-Performance Multilayer Molecular Dynamics Approaches,**  
Curso en *Quantum dynamics* (4 hours),  
Autonoma University Madrid, Spain

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## International congresses organisation

- 2026 **High Dimensional Quantum Dynamics (HDQD2026),**  
*Organising committee: Cristina Sanz Sanz and Sandra Gómez (USAL),*  
Venue: University of Salamanca, Salamanca (Spain)
- 2019 **10th International Meeting on Atomic and Molecular Physics and Chemistry (IMAMPC2019),**  
*Organising committee: Cristina Sanz Sanz, Sergio Díaz-Tendero and Daniel Arismendi Arrieta (DIPC),*  
Venue: Spanish National Research Council, Madrid (España)  
<http://imampc2019.wordpress.com>

## Oral presentations in international conferences (last 10 years)

- 2022 *Stark effect control or pulse delayed excitation/de-excitation effect in the photodissociation of IBr molecule?*  
High Dimensional Quantum dynamics (HDQD2022). Groningen (Netherlands).
- 2021 *Control of the dissociation of IBr: Stark effect or pulse delayed excitation/de-excitation effect?*  
International Chemical congress of pacific basin societies (PACIFICHEM2021). Hawái (United States of America). Virtual Conference
- 2019 *Multisheeted global fit of CBS energies of the lowest singlet and triplet states of  $H_3^+$*   
2nd meeting of the CEHISM PICS. Salamanca (Spain)
- 2019 *Field modified potential energy curves control of the dissociation branching ratio in the IBr system.*  
International Symposium on Ion-Atom Collisions (ISIAC2019). Paris (France)
- 2019 *Control of the dissociation branching ratio in the IBr system.*  
Extended software development workshops – Quantum dynamics (ESDW2019). Durham (United Kingdom)
- 2018 *IBr branching ratio using excitation and control pulses parallel to molecular axis*  
High Dimensional Quantum Dynamics (HDQD2018). Lille (France)
- 2017 *Three singlet states global fitting of  $H_3^+$  with improved Long-Range description*  
8th International Meeting on Atomic and Molecular Physics and Chemistry (IMAMPC2017). Torun (Poland)
- 2017 *Control of the dissociation branching ratio in the IBr system*  
4th XLIC General meeting. Prague (Czech Republic)
- 2015 *New improvements in the description of the PES and collisions of  $H_2 + H_2^+$  system*  
XIII Iberian Joint Meeting on Atomic and Molecular Physics (IBER2015). Aveiro (Portugal)
- 2015 *New improvements in the description of the PES and collisions of  $H_2 + H_2^+$  system*  
6th International Meeting on Atomic and Molecular Physics and Chemistry (IMAMPC2015). Birmingham (United Kingdom)
- 2015 *New improvements in the description of the PES and collisions of  $H_2 + H_2^+$  system*  
13th International workshop on Quantum Reactive Scattering (QRS2015). Salamanca (Salamanca)
- 2014 *Quantum study and quasi-classical collisions of  $H_2 + H_2^+$  reaction*  
5th International Meeting on Atomic and Molecular Physics and Chemistry (IMAMPC2014). Salamanca (Spain)
- 2014 *LS depolarizing transitions in A+H collisions: a diabaticization approach*  
Theory and modelling of polarisation in astrophysics - WG2 meeting. Praga (Czech Republic)
- 2014 *Quantum Dynamics studies on the Strong Field Control of IBr*  
Control of Chemical Reactivity 2014 - WG3 meeting. Birmingham (United Kingdom)

## Seminars

- 2018 *IBr branching ratio using excitation and control pulses parallel to molecular axis*  
Universidad de Groningen, Groningen (Netherlands)
- 2012 *Dynamics and control of the photodissociation of NH<sub>3</sub> and IBr. Potential energy surface of the ground state of H<sub>4</sub><sup>+</sup> system. Preliminary results of H<sub>2</sub> + H<sub>2</sub><sup>+</sup>*  
Complutense University Madrid, Madrid (Spain)
- 2009 *Analytical design of laser pulses for the alignment of the H<sub>2</sub> molecule. Optimal control of the photodissociation of the NH<sub>3</sub> molecule. Potential energy surfaces of the IBr system within the ENBO approximation*  
National Research Council, Ottawa (Canada)
- 2007 *Dynamical calculations in reactive collisions and photoinitiated processes*  
University of Bristol, Bristol (United Kingdom)
- 2005 *Probing ground and excited electronic states of LiHF and CaHCl systems to understand the harpoon mechanisms in collision and photoinitiated processes*  
Laboratoire Francis Perrin, CNRS, Paris (France)
- 2004 *CaHCl and LiHF systems: electronic structure and brief description of the stereodynamics of the reactive collision in the ground electronic state*  
Universidad de Roma "La Sapienza", Roma (Italy)