Cristina Sanz Sanz

Curriculum Vitae

Associate Professor
Departament of Applied Physical Chemistry
Autonoma University Madrid, Spain
email: cristina.sanz@uam.es

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

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

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

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: Dar. 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 Prosmiti

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 Prosmiti

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

Publications (last 10 years)

1. 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 $H_2 + H_2^+ \rightarrow H_3^+ + H$ reaction: application to plasma modelling. *Mol. Phys.*, 122:e2183071, 1 2024.

2. J. Hernández-Rodríguez, C. Sanz-Sanz, P. Alberto Enríquez, M. González, and M. Paniagua. Potential energy surfaces for singlet and triplet states of the LiH_2^+ system and quasi-classical trajectory cross sections for $H + LiH^+$ and $H^+ + LiH$. *Phys. Chem. Chem. Phys.*, 25:28052, 2023.

3. 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 NCN $^3\Sigma^-$ and CNN $^3\Sigma^-$ in astrophysical environments. *Phys. Chem. Chem. Phys.*, 25:30330, 2023.

4. J. Alonso de la Fuente, C. Sanz-Sanz, L. González-Sánchez, E. Yurtsever, R. Wester, and F. A. Gianturco. The CH^- $^3\Sigma^+$ anion: Inelastic rate coefficients from collisions with he at interstellar conditions. *J. Phys. Chem. A*, 127:765, 2023.

5. 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.

6. J. Alonso De La Fuente, C. Sanz-Sanz, L. Gonzalez-Sanchez, E. Yurtsever, R. Wester, and F. A. Gianturco. The 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 $H + H_2^+ \rightarrow H_2 + H^+$ 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 $H + D_2^+$ 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 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 $D + H_3^+ \rightarrow H_2D^+ + H$ 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 H_n^+ systems: Application to $H_2 + H_2^+ \rightarrow H + H_3^+$. *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

2024 **University College London, United Kingdom**,
Research visit to the group of Prof. Graham A. Worth,
Duration: 3 months

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.[a] Nadja Dŏslić,
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

Courses in scientific schools

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

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 Kigdom)

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 diabatization 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_3 and IBr. Potential energy surface of the ground state of H_4^+ system. Preliminary resulst of $H_2 + H_2^+$*
Complutense University Madrid, Madrid (Spain)

2009 *Analytical design of laser pulses for the alignment of the H2 molecule. Optimal control of the photodissociation of the NH3 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)