Ernesto Quintas-Sánchez **September 2, 1983. Media Luna, Cuba**

Missouri University of Science and Technology quintassancheze@mst.edu
Department of Chemistry, 104 Schrenk Hall (+1) 573 341-4451
400 W. 11th St., Rolla, MO 65409-0010.

EDUCATION

2008–12 PhD in Chemical-Physics, Bordeaux 1 University, France : *Mention "Très Honorable"* (*Summa Cum Laude*).
Dissertation : "Theoretical description of Eley–Rideal reaction dynamics on Nitrogen recombination over Tungsten surfaces".
Supervisors : Prof. Jean-Claude Rayez and Prof. Jesús Rubayo-Soneira.

2008–10 Master in Nuclear Physics, Higher Institute of Technologies and Applied Sciences (InSTEC), Cuba : *Mention "Excelente"* (*Summa Cum Laude*).
Supervisors : Dr. Pascal Larregaray, Prof. Cedric Crespos, and Prof. Jesús Rubayo-Soneira.

2002–07 Bachelor in Nuclear Physics, InSTEC, Cuba : *Mention "Título de Oro"* (*Summa Cum Laude*).
Supervisor : Prof. Jesús Rubayo-Soneira.

PROFESSIONAL EXPERIENCE

2020– *Assistant Research Professor* , Missouri University of Science and Technology, Rolla, Missouri, USA.

2017–20 *Postdoctoral Research Fellow*, Missouri University of Science and Technology, Rolla, Missouri, USA.

2015–16 *Postdoctoral Research Fellow*, LERMA, CNRS, Observatory of Paris, Meudon, France.

2012–15 *Assistant Professor*, General Physics and Mathematics Department (courses: *Methods of Mathematical Physics, Linear Algebra and Classical Mechanics*), InSTEC, Havana, Cuba.

2011–12 *Instructor Professor*, General Physics and Mathematics Department (courses: *Methods of Mathematical Physics and Mathematical Analysis*), InSTEC, Havana, Cuba

2007–11 *Teaching Assistant*, General Physics and Mathematics Department (courses: *Methods of Mathematical Physics and Optics*), InSTEC, Havana, Cuba.

2003–07 *Assistant student*, General Physics and Mathematics Department (courses: *Classical Mechanics, Optics and Electromagnetism*), InSTEC, Havana, Cuba.

RESEARCH FIELDS

Photodissociation processes on Van der Waals complexes · Molecular Dynamic Simulations · Molecular recombination on gas-surface interfaces · Quasi-classical methodology · Automated construction of Potential Energy Surfaces

SCIENTIFIC PUBLICATIONS & COMMUNICATIONS

Thesis

1. E. Quintas-Sánchez, "Theoretical description of Eley–Rideal reaction dynamics on Nitrogen recombination over Tungsten surfaces." *PhD Thesis*, Bordeaux 1 University, France (2012).

Book Chapters and Manuals

2. E. Quintas-Sánchez and R. Dawes. "AUTOSURF program: User's Guide." *In preparation* (2026).

1. R. Dawes and E. Quintas-Sánchez. "The Construction of Ab Initio-Based Potential Energy Surfaces." in *Reviews in Computational Chemistry*, eds. A. L. Parrill and K. B. Lipkowitz, Chapter 5, pp 199–264, John Wiley & Sons (2018).

Refereed Journal Publications

45. A. Batista-Planas, E. Quintas-Sánchez and R. Dawes. "Long-Range Fit: A Software Package for the Representation and Study of Long-Range Molecular Interactions." *Journal of Chemical Theory and Computation 22*, 1363–1380 (2026).

44. F. Tonolo, E. Quintas-Sánchez, A. Batista-Planas, R. Dawes and F. Lique. "Collisional Excitation of HCN by CO to Refine the Modeling of Cometary Comae." *The Journal of Physical Chemistry A 129*, 9583–9590 (2025).

43. A. Godard Palluet, R. Dawes, E. Quintas-Sánchez, A. Batista-Planas and F. Lique. "A promising statistical approach for studying the collisional excitation induced by CO: Application to the CS–CO system." *The Journal of Chemical Physics 162*, 241101 (2025).

42. D. Bostan, B. Mandal, C. Joy, M. Żółtowski, F. Lique, J. Loreau, E. Quintas-Sánchez, A. Batista-Planas, R. Dawes and D. Babikov. "Mixed quantum/classical calculations of rotationally inelastic scattering in the CO + CO system: a comparison with fully quantum results." *Physical Chemistry Chemical Physics 26* 6627–6637 (2024).

41. M.-L. Dubernet, E. Quintas-Sánchez, *et al*. "BASECOL2023 scientific content." *Astronomy & Astrophysics 683*, A40 (2024).

40. H. T. Tela, E. Quintas-Sánchez, M.-L. Dubernet, Y. Scribano, R. Dawes, F. Gattie and S. Ndengué. "Rovibrational states calculations of the H_2O–HCN heterodimer with the multiconfiguration time dependent Hartree method." *Physical Chemistry Chemical Physics 25*, 31813–31824 (2023).

39. A. Olejnik, H. Jóźwiak, M. Gancewski, E. Quintas-Sánchez, R. Dawes and P. Wcisło. "Ab initio quantum scattering calculations and a new potential energy surface for the HCl($X^1\Sigma^+$)–O_2($X^3\Sigma_g^-$) system: Collision-induced line shape parameters for O_2-perturbed R(0) 0–0 line in $H^{35}Cl$." *The Journal of Chemical Physics 159*, 134301 (2023).

38. S. Ndengué, E. Quintas-Sánchez, R. Dawes, C. Blackstone and D. Osborn. "Temperature dependence of the electronic absorption spectrum of NO_2." *The Journal of Physical Chemistry A 127*, 6051–6062 (2023).

37. F. Dumouchel, E. Quintas-Sánchez, C. Balança, R. Dawes, F. Lique and N. Feautrier. "Collisional excitation of C_2H^- by H_2: New interaction potential and scattering calculations." *The Journal of Chemical Physics 159*, 134301 (2023).

36. A. Zadrożny, H. Jóźwiak, E. Quintas-Sánchez, R. Dawes and P. Wcisło. Publisher's Note: "Ab initio quantum scattering calculations for the CO–O_2 system and a new CO–O_2 potential energy surface: O_2 and air broadening of the R(0) line in CO." *The Journal of Chemical Physics 157*, 229901 (2022).

35. Y. Ajili, E. Quintas-Sánchez, B. Mehnen, P. S. Żuchowski, F. Brzęk, N. El-Kork, M. Gacesa, R. Dawes and M. Hochlaf. "Theoretical study of the CO_2–O_2 van der Waals complex: potential energy surface and applications." *Physical Chemistry Chemical Physics 24* 28984–28993 (2022).

34. A. Zadrożny, H. Jóźwiak, E. Quintas-Sánchez, R. Dawes and P. Wcisło. "Ab initio quantum scattering calculations for the CO–O_2 system and a new CO–O_2 potential energy surface: O_2 and air broadening of the R(0) line in CO." *The Journal of Chemical Physics 157*, 174310 (2022).

33. O. Denis-Alpizar, E. Quintas-Sánchez and R. Dawes. "State-to-state rate coefficients for HCS^+ in rotationally inelastic collisions with H_2 at low temperatures." *Monthly Notices of the Royal Astronomical Society 512*, 5546–5551 (2022).

32. K. Dzenis, A. Faure, B. A. McGuire, A. J. Remijan, P. J. Dagdigian, C. Rist, R. Dawes, E. Quintas-Sánchez, F. Lique and M. Hochlaf. "Collisional Excitation and Non-LTE Modeling of Interstellar Chiral Propylene Oxide." *The Astrophysical Journal 926*, 3 (2022).

31. E. Quintas-Sánchez, R. Dawes and O. Denis-Alpizar. "Theoretical study of the HCS^+–H_2 van der Waals complex: potential energy surface, rovibrational bound states, and rotationally inelastic collisional cross sections." *Molecular Physics 119*, e1980234 (2021).

30. M. Gancewski, H. Jóźwiak, E. Quintas-Sánchez, R. Dawes, F. Thibault and P. Wcisło. "Fully quantum calculations of O_2–N_2 scattering using a new potential energy surface: Collisional perturbations of the oxygen 118 GHz fine structure line." *The Journal of Chemical Physics 155*, 124307 (2021).

29. C. Balança, E. Quintas-Sánchez, R. Dawes, F. Dumouchel, F. Lique and N. Feautrier. "Inelastic rate coefficients for collisions of C_4H^- with H_2." *Monthly Notices of the Royal Astronomical Society 508*, 1148–1155 (2021).

28. S. Ndengué, E. Quintas-Sánchez, R. Dawes and D. Osborn. "The low-lying electronic states of NO_2: Potential energy and dipole surfaces, bound states, and electronic absorption spectrum." *The Journal of Physical Chemistry A 125*, 5519–5533 (2021).

27. E. Quintas-Sánchez and R. Dawes. "Spectroscopy and Scattering Studies Using Interpolated Ab Initio Potentials." *Annual Review of Physical Chemistry vol. 72*, 399–421 (2021).

26. B. Desrousseaux, E. Quintas-Sánchez, R. Dawes, S. Marinakis and F. Lique. "Collisional excitation of interstellar PN by H_2: New interaction potential and scattering calculations." *The Journal of Chemical Physics 154*, 034304 (2021).

25. C. Bop, E. Quintas-Sánchez, S. Sur, M. Robin, F. Lique and R. Dawes. "Inelastic scattering in isotopologues of O_2–Ar: the effects of mass, symmetry, and density of states." *Physical Chemistry Chemical Physics 23* 5945–5955 (2021).

24. B. Desrousseaux, F. Lique, J. Goicoechea, E. Quintas-Sánchez and R. Dawes. "CF^+ excitation in the interstellar medium." *Astronomy & Astrophysics 645*, A8 (2021).

23. C. Bop, F. Lique, A. Faure, E. Quintas-Sánchez and R. Dawes. "Non-LTE modelling of cyanoacetylene: evidence for isomer-specific excitation." *Monthly Notices of the Royal Astronomical Society 501*, 1911–1919 (2021).

22. M. Khalifa, E. Quintas-Sánchez, R. Dawes, K. Hammami and L. Wiesenfeld. "Rotational quenching of an interstellar gas thermometer: CH_3CN–He collisions." *Physical Chemistry Chemical Physics 22*, 17494–17502 (2020).

21. E. Quintas-Sánchez, R. Dawes, X.-G. Wang and T. Carrington Jr. "Computational study of the rovibrational spectrum of CO_2–N_2." *Physical Chemistry Chemical Physics 22*, 22674–22683 (2020).

20. E. Quintas-Sánchez, R. Dawes, K. Lee and M. McCarthy. "Automated construction of potential energy surfaces suitable to describe van der Waals complexes with highly excited nascent molecules: The rotational spectra of Ar–CS(v) and Ar–SiS(v)." *The Journal of Physical Chemistry A 124*, 4445–4454 (2020).

19. S. Sur, S. Ndengué, E. Quintas-Sánchez, C. Bop, F. Lique and R. Dawes. "Rotationally inelastic scattering of O_3-Ar: state-to-state rates with the multiconfigurational time dependent Hartree method." *Physical Chemistry Chemical Physics 22*, 1869–1880 (2020).

18. M-L. Dubernet and E. Quintas-Sánchez. "First quantum study of the rotational excitation of HCN by para-H_2O: convergence of quantum results, influence of the potential energy surface, and rate coefficients of interest for cometary atmospheres." *Molecular Astrophysics 16*, 100046 (2019).

17. E. Castro-Juárez, X.-G. Wang, T. Carrington Jr., E. Quintas-Sánchez and R. Dawes. "Computational Study of the Ro-Vibrational Spectrum of CO–CO_2." *The Journal of Chemical Physics 151*, 020932 (2019).

16. B. Desrousseaux, E. Quintas-Sánchez, R. Dawes and F. Lique. "Collisional Excitation of CF^+ by H_2: Potential Energy Surface and Rotational Cross Sections." *The Journal of Physical Chemistry A 123*, 9637–9643 (2019).

15. E. Quintas-Sánchez and R. Dawes. "AUTOSURF: a Freely Available Program to Construct Potential Energy Surfaces." *Journal of Chemical Information and Modelling 59*, 262–271 (2019).

14. A. Faure, P. J. Dagdigian, C. Rist, R. Dawes, E. Quintas-Sánchez, F. Lique and M. Hochlaf. "Interaction of chiral propylene oxide (CH_3CHCH_2O) with helium: potential energy surface and scattering calculations." *ACS Earth and Space Chemistry 3*, 964–972 (2019).

13. C. Bop, F. Batista, A. Faure, E. Quintas-Sánchez, R. Dawes and F. Lique. "Isomerism Effects in the Collisional Excitation of Cyanoacetylene by Molecular Hydrogen", *ACS Earth and Space Chemistry 3*, 1151–1157 (2019).

12. S. Sur, E. Quintas-Sánchez, S. A. Ndengué and R. Dawes. "Development of a potential energy surface for the O_3–Ar system: Rovibrational states of the complex." *Physical Chemistry Chemical Physics 21*, 9168–9180 (2019).

11. E. Quintas-Sánchez and M-L. Dubernet. "Theoretical study of HCN–water interaction: five dimensional potential energy surfaces." *Physical Chemistry Chemical Physics 19*, 6849 (2017).

10. M-L. Dubernet, E. Quintas-Sánchez, *et al*. "The Virtual Atomic and Molecular Data Center (VAMDC) Consortium." *Journal of Physics B: Atomic, Molecular and Optical Physics*, *49*, 074003 (2016).

9. M-L. Dubernet, E. Quintas-Sánchez and P. Tuckey. "New potential energy surface for the HCS^+–He system and inelastic rate coefficients for the interstellar medium." *The Journal of Chemical Physics 143*, 044315 (2015).

8. R. Petuya, C. Crespos, E. Quintas-Sánchez and P. Larregaray. "Comparative Theoretical Study of H_2 Eley-Rideal Recombination Dynamics on W(100) and W(110)." *The Journal of Physical Chemistry C 118*, 11704 (2014).

7. E. Quintas-Sánchez, P. Larregaray and C. Crespos. "Influence of Surface Symmetry on the Onset of Nitrogen Eley-Rideal Recombination on Tungsten." *The Journal of Physical Chemistry C 118*, 12224 (2014).

6. E. Quintas-Sánchez, P. Larregaray, C. Crespos and A. Pérez Mellor. "Estudio teórico del mecanismo Eley-Rideal en la recombinación de nitrógeno sobre tungsteno (110)." *Revista Cubana de Física 30*, 66 (2013).

5. E. Quintas-Sánchez, C. Crespos, P. Larregaray, L. Martin Gondre, J. Rubayo-Soneira and J. C. Rayez. "Surface temperature effects on the energetics of N_2 molecules formed by Eley-Rideal recombination on W(100)." *The Journal of Chemical Physics 138*, 024706 (2013).

4. E. Quintas-Sánchez, P. Larregaray, C. Crespos, L. Martin Gondre, J. Rubayo-Soneira and J. C. Rayez. "Dynamical reaction pathways in Eley-Rideal recombination of nitrogen from W(100)." *The Journal of Chemical Physics 137*, 064709 (2012).

3. L. Barrios Herrera, E. Quintas-Sánchez, L. Martin, C. Crespos, P. Larregaray, J. C. Rayez and J. Rubayo-Soneira. "Sección eficaz Eley–Rideal en la recombinación de nitrógeno sobre W(100)." *Revista Cubana de Física 28*(1E), 61-65 (2011).

2. E. Quintas-Sánchez, P. Larregaray, C. Crespos, L. Martin Gondre, J. Rubayo-Soneira and J. C. Rayez. "Dinámica Eley-Rideal vs átomos-calientes en la recombinación de Nitrógeno sobre W(100)." *Revista Cubana de Física 27*(2B), 244-250 (2010).

1. J. L. Borrel, N. López-Pino, O. Díaz Rizo, K. D'Alessandro, F. Padilla, Y. Arbelo, A. Garcia, E. Quintas-Sánchez and A. O. Casanova. "Uranium enrichment determination of the InSTEC sub-critical ensemble fuel by gamma spectrometry." *Nucleus 45*, 37-43 (2009).

Conference Papers

9. E. Quintas-Sánchez, R. Dawes, K. Lee and M. McCarthy. "The Automated Construction of Potential Energy Surfaces Suitable to Describe vdW Complexes of Highly Excited Nascent Reaction Products Molecules." *74rd ISMS*, Champaign-Urbana, Illinois USA, DOI: 10.15278/isms.2019.TH06 (2019).

8. R. Dawes, E. Quintas-Sánchez, K. Lee and M. McCarthy. "The Prediction and Observation of vdW Complexes of Highly Vibrationally Excited CS and SiS with Ar." *74rd ISMS*, Champaign-Urbana, Illinois USA, DOI: 10.15278/isms.2019.TH07 (2019).

7. S. Sur, S. Ndengué, E. Quintas-Sánchez and R. Dawes. "Inelastic Collision Dynamics of O_3 + Ar." *74rd ISMS*, Champaign-Urbana, Illinois USA, DOI: 10.15278/isms.2019.RJ08 (2019).

6. B. Welch, E. Quintas-Sánchez and R. Dawes. "Evaluating VPT2 Schemes for Accurate Automated Thermochemistry and Spectroscopy for Non-Covalent Systems." *74rd ISMS*, Champaign-Urbana, Illinois USA, DOI: 10.15278/isms.2019.WD05 (2019).

5. E. Quintas-Sánchez and R. Dawes. "Autosurf: a Code for Automated Construction of Potential Energy Surfaces." *Abstracts of papers of the American Chemical Society (vol. 256)*, National Meeting of the ACS, Division of Physical Chemistry, Session: From Potential Energy Surfaces to Dynamics & Kinetics, paper id: 2980227 (*PHYS 28*), Boston USA, (2018).

4. S. Sur, E. Quintas-Sánchez, S. Ndengué and R. Dawes. "Inelastic Collisions of Ar and O_3." *Abstracts of papers of the American Chemical Society (vol. 256)*, National Meeting of the ACS, Division of Physical Chemistry, Session: From Potential Energy Surfaces to Dynamics & Kinetics, paper id: *PHYS 176*, Boston USA, (2018).

3. E. Quintas-Sánchez and R. Dawes. "Autosurf: a Code for Automated Construction of Potential Energy Surfaces." *73rd ISMS*, Champaign-Urbana, Illinois USA, DOI: 10.15278/isms.2018.RJ08 (2018).

2. S. Sur, E. Quintas-Sánchez, S. Ndengué and R. Dawes. "Inelastic Collisions of Ar and O_3." *73rd ISMS*, Champaign-Urbana, Illinois USA, DOI: 10.15278/isms.2018.RJ05 (2018).

1. E. Quintas-Sánchez and R. Dawes. "A Code for Automated Construction of Potential Energy Surfaces for van der Waals Systems." *72nd International Symposium on Molecular Spectroscopy (ISMS)*, Champaign-Urbana, Illinois USA, DOI: 10.15278/isms.2017.WI10 (2017).

CONFERENCES • WORKSHOPS • SEMINARIES

2025 - Dynamics of Molecular Collisions (DMC) Conference, Snowbird, Utah, USA.

2023 - Dynamics of Molecular Collisions (DMC) Conference, Snowbird, Utah, USA.

2019 - International Symposium on Molecular Spectroscopy (ISMS), Champaign-Urbana, Illinois, USA.

2018 - International Symposium on Molecular Spectroscopy (ISMS), Champaign-Urbana, Illinois, USA.

- American Chemical Society National Meeting, Boston, Massachusetts, USA.

2017 - International Symposium on Molecular Spectroscopy (ISMS), Champaign-Urbana, Illinois, USA.

2016 - 1st Molecules in Motion (MOLIM) Training School: From potentials to dynamic, Curia, Portugal.

2015 - Journées Scientifiques du GDR ThéMS (*Théorie, Modélisation, Simulation*), Orsay, France.

- 13th International Workshop on Quantum Reactive Scattering, Salamanca, Spain.

2012 - 2nd Workshop on Atomic and Molecular Physics. Varadero, Cuba.

- Seminar at ICIMAF, Havana, Cuba.

2011 - XII Simposio de la Sociedad Cubana de Física. Havana, Cuba.

2010 - VI International Meeting on Photodynamics. Havana, Cuba.

- Journée Scientifique du ISM, Talence, France.

- Passion for Knowledge, Donostia - San Sebastian, Spain.

- International Meeting on Atomic and Molecular Physics and Chemistry (IMAMPC), Madrid, Spain.

2009 - Seminar at CSIC, Madrid, Spain.

- 1st Workshop on Atomic and Molecular Physics. Havana, Cuba.

- XII Workshop on Nuclear Physics and VI International Symposium on Nuclear-Related Techniques. Havana, Cuba.

- Journée Dynamique du Sud Ouest (JDSO), Talence, France.

- XIV International Workshop on Quantum Systems in Chemistry and Physics (QSCP), Madrid, Spain.

2008 - V International Meeting on Photodynamics. Havana, Cuba.

2007 - XXXIII Congreso de Químicos Teóricos de Expresión Latina (QUITEL). Havana, Cuba.

AWARDS

2013 Prize *Outstanding Scientific Result* by InSTEC, Cuba.

2013 Professor *Tiza de Oro*, InSTEC, Cuba.

2008 Grant from the French Embassy in Cuba for an International Joint Doctorate between InSTEC, Cuba, and Université Bordeaux 1, France.

2007 Prize *Best Academic Graduated* by InSTEC, Cuba.

2001 Gold Medal, Iberoamerican Physics Olympiad. Sorata, Bolivia.

PROFESSIONAL MEMBERSHIPS AND ASSOCIATIONS

American Chemical Society / Member, 2018–present.

Cuban Physics Society / Member, 2011–present.

LANGUAGES

Spanish Fluent (native language).

English Excellent.

French speech: regular, reading: good, writing: elementary.

REFERENCES

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