



# Ramón L. PANADÉS-BARRUETA

Ave Paul Langevin, Residence REEFLEX A316, Villeneuve d'Ascq, France

## Education

- 2017–2020 **PhD Candidate in Physics**, *Université de Lille, Laboratoire de Physique des Lasers, Atomes et Molécules (PhLAM)*, France.  
Thesis title: Full quantum simulations of the interaction between atmospheric molecules and model soot particles  
Supervisor: Prof. Dr. Daniel PELÁEZ-RUIZ ([ISMO](#), Université Paris-Saclay)
- 2016–2017 **MSc in Physics (International Master 2 Atmospheric Environments)**, *Université de Lille, Laboratoire de Physique des Lasers, Atomes et Molécules (PhLAM)*, France.  
**Distinction: Mention Bien**  
Thesis title: Towards a quantum dynamical description of the photodissociation of  $Cl_2$  molecule adsorbed on ice  
Supervisors: Prof. Dr. Daniel PELAEZ-RUIZ and Prof. Dr. Maurice MONNERVILLE
- 2011–2016 **BSc in Radiochemistry**, *University of Havana, Higher Institute of Technologies and Applied Sciences (InSTEC)*, Havana, Cuba.  
**Distinction: Summa Cum Laude**  
Thesis title: Mean Potential Phase Space Theory study of the  $Si(^3P) + OH(X^2\Pi) \rightarrow SiO(X^1\Sigma^+) + H(^2S)$  reaction  
Supervisor: Dr. Alejandro RIVERO-SANTAMARÍA ([CMF](#), Universidad del País Vasco)

## Publications

- 2020 Panadés-Barrueta, R. L. and Peláez, D. **Low-Rank Sum-of-Products Finite-Basis-Representation (SOP-FBR) of Potential Energy Surfaces**, *The Journal of Chemical Physics*, *in review*
- 2019 Panadés-Barrueta, R. L., Martínez-Núñez, E., & Peláez, D. (2019). **Specific Reaction Parameter Multigrid POTFIT (SRP-MGPF): Automatic Generation of Sum-of-Products Form Potential Energy Surfaces for Quantum Dynamical Calculations**, *Frontiers in Chemistry*, **7**, 576. Included in the book [Application of Optimization Algorithms in Chemistry](#)
- 2016 Panadés-Barrueta, R. L., Rubayo-Soneira, J., Monnerville, M., Larregaray, P., Dayou, F., & Rivero-Santamaría, A. (2016). **Mean Potential Phase Space Theory study of the  $Si(^3P) + OH(X^2\Pi) \rightarrow SiO(X^1\Sigma^+) + H(^2S)$  reaction**, *Revista Cubana de Física*, **33(2)**, 102-117.

## Seminars and conferences

- August 2020 **On the automatic computation of global (intermolecular) potential energy surfaces for quantum dynamical simulations**, *Invited Speaker*.  
[Symposium and Summer School on Physics of Ionized Gases](#)  
Šabac, Serbia
- February 2020 **Automatic computation of global (intermolecular) potential energy surfaces for (non) covariantly bound systems**, *Contributed Talk*.  
[Journée Chimie Théorique et Simulation Moléculaire IdF/Nord](#)  
Chimie ParisTech. Paris, France

## Teaching experience

- 2018–2019 **Laboratory of Thermodynamics.**  
Place: IUT A de Lille (Université de Lille), France   No. hours: 64   Language: French
- 2013–2016 **Math Analysis and Linear Algebra.**  
Place: InSTEC, Cuba   No. hours: 72   Language: Spanish

## Honors and Awards

- 2019 **Best Poster Prize** 10<sup>th</sup> International Meeting on Atomic and Molecular Physics and Chemistry (IMAMPC). Madrid, Spain.
- 2018 **Best Poster Prize** 6<sup>th</sup> High Dimensional Quantum Dynamics Workshop (HDQD). Lille, France.
- 2018 **PCCP Best Poster Prize** 9<sup>th</sup> International Meeting on Atomic and Molecular Physics and Chemistry (IMAMPC). Berlin, Germany.
- 2015 **ICPC Contestant** Caribbean Finals of the International Collegiate Programming Contest (ACM-ICPC). Havana, Cuba
- 2010 **IChO Contestant** Captain of the Cuba Team in the 42<sup>nd</sup> International Chemistry Olympiad ([IChO 2010](#)). Tokyo, Japan

## Competitive research grants and fellowships

- Oct.-Dec. **Research Grant German Academic Exchange Service (DAAD).**  
2019 Awarded by: Deutscher Akademischer Austausch Dienst  
Place: Universität Heidelberg, Theoretical Chemistry Group  
Supervisor: Prof. Dr. Oriol VENDRELL
- 2016–2017 **Labex CaPPA Fellowship.**  
Awarded by: Laboratoire d'excellence CaPPA  
Place: Université de Lille

## Research training

- August 2019 **School EMIE-UP. Multiscale Dynamics in Molecular Systems**, *École de Physique des Houches. Haute-Savoie, France.*
- June 2019 **3<sup>rd</sup> Mini-school on mathematics for theoretical chemistry and physics**, *Sorbonne Université, Pierre et Marie Curie. Paris, France.*
- June 2018 **Bridging experiment and theory in precision spectroscopy (BETS) 4<sup>th</sup> MOLIM Training School**, *Nicolaus Copernicus University. Torun, Poland.*
- January 2018 **Label of Theoretical Chemistry Île de France-Nord**, *Sorbonne Université, Pierre et Marie Curie. Paris, France.*
- October 2017 **Quantum Dynamics with the Multi-Configuration Time-Dependent Hartree (MCTDH) method: future and perspectives**, *Université Paris-Saclay. Paris, France.*

## Computer skills

- OS UNIX, ([Arch](#)) Linux, Android
- Languages Python (SciPy, NumPy, Matplotlib), C, FORTRAN, Bash, Lisp, Julia,  $\text{\LaTeX}$
- Software [MCTDH](#) (Developed the SOP-FBR and SRPTucker packages), MOPAC, MOLPRO, MOLCAS, Gaussian, [AutoMeKin](#), Inkscape, Git

## Languages (CEFR)

- Spanish Native speaker
- English Proficient user (C1)
- French Proficient user (C1)
- German Basic user (A1)