



# Ramón L. PANADÉS-BARRUETA

## Curriculum Vitae

### Professional experience

- 2020–Present **Postdoctoral fellow**, [University of Twente](#), Computational Chemical Physics Group ([CCP](#)), Netherlands.  
Project: Targeting Real chemical accuracy at the EXascale ([TREX](#)). European HPC Centre of Excellence ([CoE](#))

### Education

- 2017–2020 **PhD in Physics**, [University of 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 (available at [theses.fr](#))  
Supervisor: Prof. Dr. Daniel PELÁEZ-RUIZ ([ISMO](#), Université Paris-Saclay)
- 2016–2017 **MSc in Physics (International Master 2 Atmospheric Environments)**, [University of Lille](#), Laboratoire de Physique des Lasers, Atomes et Molécules ([PhLAM](#)), France.  
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.  
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

- 2021 Panadés-Barrueta, R. L., D. Duflot, K. Dembele and Peláez, D. **Automatic vdW-TSSCDS determination of the physisorbed stationary points of the NO<sub>2</sub>-Pyrene van der Waals cluster in full dimensionality**, *Journal of Physical Chemistry A*, in preparation.
- 2020 Panadés-Barrueta, R. L. and Peláez, D. (2020). **Low-Rank Sum-of-Products Finite-Basis-Representation (SOP-FBR) of Potential Energy Surfaces**, *Journal of Chemical Physics*, **153**, 234110.
- 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., and Rivero-Santamaría, A. (2016). **Mean Potential Phase Space Theory study of the Si(<sup>3</sup>P) + OH(X<sup>2</sup>Π) → SiO(X<sup>1</sup>Σ<sup>+</sup>) + H(<sup>2</sup>S) 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) covalently bound systems**, *Contributed Talk*.

Journée Chimie Théorique et Simulation Moléculaire IdF/Nord  
Chimie ParisTech. Paris, France

## Teaching experience

2021 **Qualification for a position as an assistant professor in a French University.**

Sections: 30 and 31 of the CNU Qualification Numbers: 21230359242 and 21231359242

2018–2019 **Laboratory of Thermodynamics.**

Place: IUT A de Lille (University of Lille), France No. hours: 64 Language: French

2013–2016 **Math Analysis and Linear Algebra.**

Place: InSTEC (University of Havana), 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: University of 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

Numerical methods Tensor decomposition, Optimization Algorithms, Quantum Monte Carlo, HPC optimization

## Languages (CEFR)

- Spanish Native speaker
- English Proficient user (C1)
- French Proficient user (C1)
- German Basic user (A2)