



# Ramón L. PANADÉS-BARRUETA

[panadestein.github.io](https://panadestein.github.io)

## 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  $\text{Si}({}^3\text{P}) + \text{OH}({}^2\Pi) \rightarrow \text{SiO}({}^1\Sigma^+) + \text{H}({}^2\text{S})$  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 (proficient in SciPy ecosystem), C, FORTRAN, Bash, Lisp, Julia, L<sup>A</sup>T<sub>E</sub>X, HTML/CSS
- Software Wolfram Mathematica, Emacs, Git, [MCTDH](#) (Developed the SOP-FBR and SRPTucker packages), [CHAMP](#), [AutoMeKin](#), MOPAC, MOLPRO, MOLCAS, Gaussian, Inkscape, Libreoffice
- 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, Goethe-Institut certified) |