



# Dr. Ernesto García Alfonso

November 14<sup>th</sup>, 1996

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Skills

Spanish (mother tongue)

English (B2)

French (B1)

Technical skills

- UNIX (UBUNTU)
- Fortran 90, C++, Python, GIT-HUB, HTML, MPI, OpenMP
- Supercomputer center (CALMIP, Toulouse) <https://www.calmip.univ-toulouse.fr/>
- Latex

## About me

During my free time, I like reading mystery and fiction books and practising some sports such as football, volleyball and biking. I like to spend time with my family and friends. I enjoy team work.

## Postdoc

Pisa, Italy:

September 2024  
"Simulation from prime principles of structure and optical properties and Catalysts of metal nano aggregates". Area della Ricerca del CNR di Pisa

## Education

PhD:
October 2021-May 2024

Title: *Theoretical study of superfluid helium nanodroplet dynamics: cluster formation, ion solvation, Coulomb explosion, quantum vortex nucleation and detection.*  
Lab: Laboratoire Collisions Agrégats Réactivité (LCAR) Toulouse, France  
Thesis advisor: Nadine Halberstadt

2015–2020

Master in physics. Havana University (Cuba), Physics Faculty. Title: *"Study of the Vibrational Predissociation of the NeBr<sub>2</sub> Complex by Computational Simulation Using the Trajectory Surface Hopping Method"*.  
Thesis advisor: Maykel Marquez Mijares and Jesús Rubayo Soneira

## Conferences

Participation in national/international Conferences [Poster (4/6) and Oral Presentation (5/10)]  
[https://github.com/ErnestoGarciaALfonso/Experience/blob/main/Professional\\_experience.pdf](https://github.com/ErnestoGarciaALfonso/Experience/blob/main/Professional_experience.pdf)



## Publications

In international journals with peer review (10) <https://github.com/ErnestoGarciaALfonso/List-of-Papers/blob/main/Papers.pdf>

## Grants

April-2024 NANO X (nanoscale science and engineering). PhD student mobility

## Membership

2023 Confined Molecular Systems: From a new Generation of Materials to the Starts (COSY) Work Group 4

## Stay Abroad

★[07/2019–10/2019] Participation. Project "Theoretical study of helium nanodroplets dynamics: alkali dopants and quantum Vortex; rare gas dopants and cluster formation" in Toulouse, France. Participants: Nadine Halberstadt, Manuel Barranco and Martí Pi from University of Barcelona. Spain

★[04/03-27/2024] "Photodissociation of Ak<sub>2</sub> induced by the helium environment. A DIM (Diatomics in Molecules) model to describe the interactions between the dialkali and the <sup>4</sup>He<sub>N</sub> nanodroplet and the couplings between the electronics tates of the dialkali molecule induced by helium". Consejo Superior de Investigaciones Científicas(CSIC), Madrid Spain.

## Publications

- 2024 Marisol Trejo, Andrew Clifford, Ernesto Garcia Alfonso, Nadine Halberstadt, Lan Xue, and Wei Kong. "*Electron diffraction of foam-like clusters between xenon and helium in superfluid helium droplets*" J. Chem. Phys. 161, 000000 (2024)
- Ernesto García-Alfonso, Manuel Barranco, Nadine Halberstadt and Martí Pi. "*Time-resolved solvation of alkali ions in superfluid helium nanodroplets*". J. Chem. Phys. 160, 164308 (2024)
- Loidel Puentes-Milián, Ernesto Garcia-Alfonso, Maykel MARQUEZ-MIJARES, and Jesús Rubayo-Soneira. "*Vibrational predissociation study of NeIBr(A) using Quasiclassical Trajectories and Trajectory Surface Hopping methods*". Chemical Physics Letters. 849, 141427 (2024)
- 2023 Loidel Puentes-Milián, Ernesto Garcia-Alfonso, Maykel MARQUEZ-MIJARES, and Jesús Rubayo-Soneira. "*NeI2 Photofragmentation Dynamics Through Quasiclassical and Semiclassical Studies*". ChemPhysChem e202300406, 2023
- Ernesto García-Alfonso, Francesco Ancilotto, Manuel Barranco, Martí Pi, Nadine Halberstadt. "*Quantized vortex nucleation in collisions of superfluid nanoscopic helium droplets at zero temperature*". J. Chem. Phys. 159, 074305 (2023)
- 2022 Ernesto García-Alfonso, Maykel Márquez-Mijares, Jesús Rubayo-Soneira, Nadine Halberstadt, Kenneth C. Janda and Craig C. Martens. "*Photofragmentation dynamics study of ArBr<sub>2</sub> ( $\nu = 16 \dots, 25$ ) using two theoretical methods: trajectory surface hopping and quasiclassical trajectories*". Eur. Phys. J. D. 76, 79. 2022.
- Ernesto García-Alfonso, Manuel Barranco, David A. Bonhommeau, Nadine Halberstadt, Martí Pi and Florent Calvo. "*Clustering, collision, and relaxation dynamics in pure and doped helium nanoclusters: Density - vs particle -based approaches*". The Journal of Chemical Physics. 157, 014106. 2022.
- 2020 Ernesto García-Alfonso, Francois Coppens, Manuel Barranco, Martí Pi, Frank Stienkemeier and Nadine Halberstadt. "*Alkali atoms attached to vortex-hosting helium nanodroplets*". The Journal of Chemical Physics. 152, 194109. 2020.
- Ernesto García-Alfonso, Maykel Márquez-Mijares, Jesús Rubayo-Soneira, Nadine Halberstadt, Kenneth C. Janda and Craig C. Martens. "*Study of the Vibrational Predissociation of the NeBr<sub>2</sub> Complex by Computational Simulation using the Trajectory Surface Hopping Method*". Sigma Mathematics. 8, 2029. 2020.
- 2019 C. Calvo-Mola, S. López Pérez, E. García Alfonso, and J. Cerutti-Torres. "*Determination of the Planck Constants through the use of LEDs*". Revista Cubana de Física, 36, 125. 2019.



## Conferences

- 07/1-5/2024 **Oral Presentation** 24th European Conference on the Dynamics of Molecular Systems, Aarhus, Denmark.
- 06/23-26/2024 **Poster** The 15th International Conference on Quantum Fluid Clusters, Aarhus, Denmark.
- 06/18-21/2024 **I have run a section in the training school** COST COSY training school "Confined molecular systems in Helium nanodroplets" at Eli beamline, Prague, Czech Republic.
- 01/03-09/2024 **Poster** Molecular and Ionic Clusters. Gordon Research Conference (GRC). Ventura (California). United States. (Due to U.S policy aim to Cuban people I was unable to get a visa, so Nadine Halberstadt presented my poster on site )
- 07/03-07/2023 **Oral Presentation+Poster** Congrès Général des 150 ans de la Société Française de Physique. Paris, France
- 06/20-21/2023 **Poster** AtmChemClimate workshop in Montpellier. France
- 06/01-02/2023 **Oral Presentation** XVèmes Journées de l'ED. Toulouse
- 03/01-03/2023 **Oral Presentation** First COSY General Meeting, Cadiz, Spain.
  - 01/24/2023 **Oral Presentation** First meeting of the CONFINED MOLECULAR SYSTEMS: FROM A NEW GENERATION OF MATERIALS TO THE STARS (COSY), COSY Working Group 4 (Helium nanodroplets in science and engineering) (online)
  - 11/11/2022 **Poster** (online) PHOTODYNAMICS 2022, XI International Meeting of Photodynamics, La Havana, Cuba
  - 11/7-8/2022 **Oral Presentation** Les Toulousaines du Calcul Atomique et Moléculaire (TouCAM), Toulouse, France
  - 10/19/2022 **Oral Presentation** at Instituto de Física Fundamental (IFF-CSIC) Departamento de Procesos Atómicos, Moleculares y en Superficies Consejo Superior de Investigaciones Científicas, Madrid Spain. "*Coulomb Explosion of Alkali Dimers on Helium Droplets. Is Really Triplet State Dominant?*"
- 09/05-09/2022 **Participation in training school** "Machine Learning and Quantum Computing for Quantum Molecular Dynamics" (CECAM-FR-MOSER). Gustave Eiffel Université, (Paris), France.
- 08/7-12/2022 **Poster** Molecular and Ionic Clusters. Gordon Research Conference (GRC) , Lucca (Barga), Italy.
- 08/6-7/2022 **Oral Presentation** Molecular and Ionic Clusters. Gordon Research Seminar (GRS) , Lucca (Barga), Italy.
- 04/18-23/2022 **Oral Presentation + Poster** The 14<sup>th</sup> International Conference on Quantum Fluid Clusters, Erice, Sicily, Italy.
- 03/10-11/2022 **Poster** NanoX-FerMI days. Toulouse, France.
  - 11/2021 **Oral Presentation** Réunion annuelle du GDR THEMS. Toulouse, France.
  - 06/2021 **Oral Presentation** (online). XV Taller de Física de la Materia Condensada y Molecular. Cuernavaca, Morelos, Mexico.
- 10/2020–08/2021 I taught Atomic and Molecular Physics online (on-site classes were forbidden because of COVID-19) to two groups of 3rd year (20 students each)
  - 03/2020 **Poster**. XV Simposio y XIII Congreso de la Sociedad Cubana de Física. La Habana, Cuba.
- 03/11-15/2019 **Oral Presentation** VIII Taller Iberoamericano de Enseñanza de la Física Universitaria. ("Determination of the Planck Constants through the use of LEDs") La Havana, Cuba

## Conferences

- 2018 **Presentation** Scientific day ICIMAF (“Study of the Vibrational Predissociation of the NeBr<sub>2</sub> Complex by Computational Simulation using the Trajectory Surface Hopping Method”) Cuba
- 2018–2021 **Participation** . Research Project (National Basic Sciences Program). “*Study of confinement, relaxation and energy transfer processes of atomic and molecular systems*”. Department of Atomic and Molecular Physics. Higher Institute of Technologies and Applied Sciences (InSTEC), University of Havana. Cuba
- 2016–2017 **Participation**. InSTEC Research Project (Financier: InSTEC). Physico-chemical study of atomic and molecular systems with interest for the environment. Department of Atomic and Molecular Physics. Higher Institute of Technologies and Applied Sci