

# Dr. Ernesto García Alfonso

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

Pisa, Italy

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https://github.com/ ErnestoGarciaALfonso

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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

## **A** Education

PhD:

October 1<sup>st</sup> 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







#### Q 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 Halberstad, Manuel Barranco and Martí Pi from University of Barcelona. Spain

 $\star$ [04/03-27/2024] "Photodissociation of Ak $_2$  induced by the helium environment. A DIM (Diatomics in Molecules) model to describe the interactions between the dialkali and the  ${}^4$ He $_N$  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. "Photogfragmentation dynamics study of ArBr $_2$  ( $\nu=16\ldots,25$ ) 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 NeBr2 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 Constans through the use of LEDS". Revista Cubana de Física, 36, 125.2019.



- 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 Géneral 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  $14^{th}$  International Conference on Quantum Fluid Clusters, Erice, Sicily, Italy.
- 03/10-11/2022 Poster NanoX-FeRMI days. Toulouse, France.
  - 11/2021 Oral Presentation Réunion anuelle 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 Constans through the use of LEDS") La Havana, Cuba

- 2018 Presentation Scientific day ICIMAF ("Study of the Vibrational Predissociation of the NeBr2 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