CURRICULUM VITAE

Manuel Cardosa-Gutierrez

Computational scientist · PhD

EMAIL	macardosa@outlook.com
LOCATION	Houthalen-Helchteren, Belgium
CODE	codeberg.org/manuacg github.com/macardosa
STATUS	● Open to new roles

PROFILE

Computational scientist with a PhD in theoretical and computational chemistry. I build HPC software and reproducible pipelines that turn quantum-mechanical simulation into results others can check and reuse. My work spans quantum dynamics, scientific code modernisation, large datasets and containerised workflows on Linux clusters. I am looking for roles where scientific software, high performance computing and careful data work matter.

EXPERIENCE

2020–2025

Research Assistant

University of Liège, Belgium

- Developed HPC software for molecular simulation and quantum dynamics, from numerical kernels to analysis tooling.
- Ported qmd-cpp from Fortran/MKL to C++17 with an AI coding agent and validated it against the original reference output.
- Built reproducible pipelines and statistical models for large experimental and computational datasets, including smoothing, fitting and Fourier analysis.
- Managed Linux HPC clusters and deployed containerised workflows with Docker and Singularity.
- Worked with experimental colleagues to turn scientific questions into documented, repeatable workflows.

PUBLICATIONS 07

2026 Electronic coherences built by ultrashort pulse drive the vibronic forces at nonadiabatic seams
Pandey, G., Cardosa-Gutierrez, M., et al. · *Ultrafast Science* 6, 0167
doi.org/10.34133/ultrafastscience.0167

2025 Entanglement of molecular orientation and vibronic degrees of freedom by ultrafast photoexcitation in an ensemble of initially randomly oriented molecules
Cardosa-Gutierrez, M., Pandey, G., Levine, R. D., Remacle, F. · *J. Phys. Chem. Lett.* 16, 7642–7648
doi.org/10.1021/acs.jpclett.5c01729

2025 Visualizing the strong field–induced molecular breakup of C60 via x-ray diffraction
Schnorr, K., et al. · *Science Advances* 11, eadz1900
doi.org/10.1126/sciadv.adz1900

2025 Isotope effect on the few-femtosecond relaxation dynamics of the ethylene cation
Lucchini, M., Cardosa-Gutierrez, M., Murari, M., Frassetto, F., Poletto, L., Nisoli, M., Remacle, F. · *J. Phys. Chem. A* 129, 3063–3070
doi.org/10.1021/acs.jpca.5c01020

2024 Electronic coherences excited by an ultra short pulse are robust with respect to averaging over randomly oriented molecules as shown by singular value decomposition
Cardosa-Gutierrez, M., Levine, R. D., Remacle, F. · *J. Phys. Chem. A* 128, 2937–2947
doi.org/10.1021/acs.jpca.3c07856

2024 Electronic coherences built by an attopulse control the forces on the nuclei
Cardosa-Gutierrez, M., Levine, R. D., Remacle, F. · *J. Phys. B: At. Mol. Opt. Phys.* 57, 133501
doi.org/10.1088/1361-6455/ad4fd3

2023 Bond breaking of furan–maleimide adducts via a diradical sequential mechanism under an external mechanical force
Cardosa-Gutierrez, M., De Bo, G., Duwez, A.-S., Remacle, F. · *Chemical Science* 14, 1263–1271
doi.org/10.1039/d2sc05051j

EDUCATION

2020–2025

PhD, Theoretical & Computational Chemistry

University of Liège, Belgium

Stress-responsive polymers, quantum dynamics, attosecond chemistry and computational code development.

2014–2019

MSc, Radiochemistry – Summa Cum Laude

University of Havana, Cuba

AWARDS

Frédéric Swarts Prize
Royal Belgian Academy of Science · 2025

Best Poster Award
Intl. Theoretical Chemistry Symposium, IIT Madras · 2023

Best Oral Presentation
SRC Young Chemist's Day, University of Mons · 2023

SKILLS

LANGUAGES
Python · C++ · Fortran · R · SQL · Bash

SIMULATION
Gaussian · Molpro · Molcas · Q-Chem · Amber · OpenMM · SHARC

HPC & INFRASTRUCTURE
MPI · OpenMP · CUDA · Linux · Docker · Singularity · Git

DATA & AI
Pandas · NumPy · SciPy · Matplotlib · LangGraph · smolagents

LANGUAGES

Spanish	Native
English	Fluent
French	Fluent
Dutch	B1

LINKS

Codeberg
GitHub

qmd-cpp — a validated Fortran/MKL to C++17 port.

REFERENCES AVAILABLE ON REQUEST

UPDATED NOVEMBER 2026