

EVARISTO VILLASECO

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EDUCATION

Ph.D. in Theoretical Physics, *Rutgers University* | 2020–2025 | GPA: 4.0. | Best PhD Dissertation Award (University-wide).

M.Sc. in Theoretical Chemistry and Computational Modeling, *Autonomous University of Madrid* | 2016–2018 | 1 A+ Class Honor.

B.Sc. in Chemistry, *University of Salamanca* | 2012–2016 | 8 A+ Class Honors.

SKILLS & CERTIFICATIONS

Programming & Tools: Python, SQL, PySpark, Bash, AWS (EC2, S3, boto3), Git, Fortran, Flask, HPC (Slurm).

Quantitative Skills: Statistics, Probability, A/B Testing, Time Series Forecasting, Tree-based Models, NLP, GenAI.

ML & AI: PyTorch, Scikit-learn, Statsmodels, XGBoost, Hugging Face, BeeAI (AI agentic framework).

Certificates: ColumbiaX [Corporate Finance](#) (2022), Erdős Institute [Data Science](#) & [Deep Learning](#) Boot Camps (2024).

EXPERIENCE

AI Engineer | *Burnt (Internship)* | 2025–Present

- Developed a GenAI-powered WhatsApp assistant to automate order processing for sales reps, saving ~10 hours/week per rep; enabled real-time data validation using RAG and long-term memory for customer-specific context retention.
 - Designed AI workflows to automate email processing, validating purchase orders and extracting key order details for enhanced efficiency.
 - Collaborated cross-functionally with sales and product teams to align AI features with customer feedback and investor priorities.
- Tools: Python, SQL, SQLAlchemy, BeeAI, LangChain, Flask, Mem0, Twilio.

Research Scientist | *Rutgers University* | 2020–Present

- Developed a novel algorithm for molecular simulations based on coupled differential-equations, achieving 87% improvement in stability and energy conservation over standard methods. Automated large-scale simulation and data processing pipelines for 10,000+ high-dimensional trajectories across 7+ molecular systems. Integrated core contributions into open-source softwares.
Results published in: J. Chem. Phys. 158 (2023) and J. Chem. Theory Comput. 19 (2023).
- Derived a physics-informed framework and forecasting model for time-dependent molecular observables, boosting predictive accuracy by 90% over traditional modeling approaches. Designed numerical experiments to isolate the key dynamical features, enhancing signal interpretability and exposing critical limitations in conventional approaches.
Results published in: Phys. Rev. Lett. 133, 233201 (2024).
- Led an international research collaboration of 5 scientists to develop novel molecular dynamics simulation methods, resulting in 5 peer-reviewed [publications](#) in high-impact journals and 4 presentations at international conferences.
Tools: Python, Fortran, Bash, Git, HPC (Slurm).

Developer | *g-ctmqc & QuantumModelLib* | 2022–2025

- Contributed to open-source tools for molecular dynamics, expanding [g-ctmqc](#) simulation capabilities by 25% with a new simulation scheme and code optimizations, and added two quantum models to [QuantumModelLib](#), increasing modeling options by 5%.
- Tools: Python, Fortran, Bash, Git.

Machine Learning Scientist | *Burnt (Internship)* | 2024

- Developed a time-series forecasting model for restaurant sales and menu items, projecting \$250k/year savings on food costs. Performed extensive analytics uncovering key sales trends and consumer behavior to optimize inventory and menu decisions.
 - Fine-tuned LLMs (LLaMA2, BERT, GPT-2) via QLoRA, improving product categorization across food suppliers with ~92.5% accuracy.
- Tools: Python, PyTorch, Hugging Face, Statsmodels, Scikit-learn, Pandas, Seaborn.

INDEPENDENT PROJECTS

- BiteBuddy:** Built an LLM-powered nutrition assistant to deliver personalized nutrition plans leveraging tool calling and prompt engineering. Deployed on AWS (EC2, S3, Secrets Manager) for scalable, real-time access via a browser interface.
Tools: Python, Streamlit, AWS (EC2, S3, boto3, Secrets Manager) OpenAI
- LaLiga SoccerSage:** Built a Random Forest model to predict LaLiga match outcomes, outperforming bookmaker probabilities by 24%. Integrated 10+ seasons of historical match data and engineered performance metrics for a robust predictive model for sport analytics.
Tools: Scikit-learn, XGBoost, Pandas, Seaborn, Matplotlib.

PUBLICATIONS

- **E. Villaseco Arribas** and N. T. Maitra. *Phys. Rev. Lett.* **133**, 233201 (2024).
- **E. Villaseco Arribas**, N. T. Maitra, and F. Agostini. *J. Chem. Phys.* **160**, 054102 (2024).
- L. M. Ibele, E. Sangiogo Gil, **E. Villaseco Arribas**, and F. Agostini. *Phys. Chem. Chem. Phys.* (2024).
- A. Pollien, **E. Villaseco Arribas**, D. Lauvergnat, and F. Agostini. *Mol. Phys.* **0** (2024), e2378960.
- **E. Villaseco Arribas** and N. T. Maitra. *J. Chem. Phys. Commun.* **158**, 161105 (2023)
- **E. Villaseco Arribas**, L. M. Ibele, D. Lauvergnat, N. T. Maitra, and Federica Agostini. *J. Chem. Theory Comput.* **19** (2023).
- **E. Villaseco Arribas**, P. Vindel-Zandbergen, S. Roy, and N. T. Maitra. *Phys. Chem. Chem. Phys.* **25**, 26380 (2023).
- **E. Villaseco Arribas**, F. Agostini, and N. T. Maitra. *Molecules* **27** (2022), p. 13.
- A. Emelianova, E. A. Basharova, A. L. Kolesnikov, **E. Villaseco Arribas**, E. V. Ivanova and G. Y. Gor. *J. Phys. Chem. B* **125**, 16, 4086-4098 (2021).
- A.L. Ruiz, **E. Villaseco Arribas** and K. McEnnis. *Mater. Adv.*, **3**, 2858-2870 (2022).

SPEAKING ENGAGEMENTS AND CONFERENCES

American Conference in Theoretical Chemistry (ACS) | New Orleans, LA, USA (2024)

Seminar Series, Universidad de Salamanca | Salamanca, Spain (2023)

CECAM Workshop | Lausanne, Switzerland (2022)

American Conference in Theoretical Chemistry (ACS) | Palisades Tahoe, CA, USA (2022)

American Conference in Theoretical Chemistry (ACS) | Palisades Tahoe, CA, USA (2022)

Seminar Series, Université Paris Saclay | Paris, France (2022)

ACS Northeastern Regional Meeting | Rochester, NY, USA (2022)

AWARDS

Outstanding Dissertation Award | *Rutgers University* | 2025

Awarded for the best dissertation of Rutgers University in 2025, with recognition in the Hooding Ceremony program, a monetary price, and a place on a commemorative plaque.

Chateaubriand Fellowship | *Embassy of France in the United States* | 2023

Awarded a prestigious fellowship to lead a joint research project between Université Paris-Saclay and Rutgers University that resulted in 5 peer-reviewed publications.

Dean Dissertation Fellowship | *Rutgers University* | 2023

Awarded a year-long fellowship to support the completion of my dissertation, recognizing exceptional research contributions in physics.

ICIQ Summer Fellowship | *Institute of Chemical Research of Catalonia* | 2016

Ranked in the top 1.4% among 1,000+ applicants for a prestigious research program in one of Spain's leading chemical institutions.

IFIMAC Grant | *Institute of Condensed Matter Physics* | 2016

Awarded a full-tuition M.Sc. scholarship and living stipend for outstanding academic performance.