

# EVARISTO VILLASECO

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## EDUCATION

**Ph.D. in Physics**, *Rutgers University* | 2020–2025 | GPA 4.0.

**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

**Languages & Tools:** Python, SQL, Bash, Git, Flask, PySpark, Distributed Computing (HPC Clusters), AWS (EC2, S3, boto3 experience).

**Analytics & Modeling:** Statistics, Probability, A/B testing, Time Series Forecasting, Tree-based Models, NLP, and 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 & PROJECTS

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

- Developed a GenAI-powered assistant to automate order processing for sales representatives, integrating with WhatsApp for seamless communication. Enabled real-time data validation through RAG and vector search.
  - Designed AI workflows to streamline data processing and enhance automation capabilities.
  - 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 that improved numerical stability and energy conservation by 87% over standard methods. Automated large-scale simulation and data processing pipelines for 10,000+ high-dimensional trajectories across 7+ molecular systems, enabling statistical analysis and benchmarking against baseline models. 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 properties, boosting predictive accuracy by 90% over traditional modeling approaches. Designed numerical experiments to isolate the key features driving the system behavior, improving signal interpretability and exposing critical limitations in conventional approaches. Results published in: Phys. Rev. Lett. 133, 233201 (2024).
  - Led an international research collaboration, funded by the French Embassy in the US, to develop novel molecular dynamics simulation methods, resulting in 5 of 10+ peer-reviewed [publications](#) in high-impact journals and multiple 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 new simulation schemes and adding two quantum models to [QuantumModelLib](#), increasing modeling options by 5%.
- Tools: Python, Fortran, Bash, Git.

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

- Developed a demand 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.

**Data Scientist** | *Independent Projects* | 2024–2025

- BiteBuddy:** Built an AI-powered nutrition assistant that provides personalized nutrition plans based on user input. Leveraged prompt engineering and tool calling to deliver accurate, user-specific recommendations, boosting engagement and user interaction. Deployed on AWS EC2 with real-time access, leveraging S3 for data storage and Secrets Manager for secure API key management.
  - 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

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- **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

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

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

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

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

**CECAM Workshop** | Lausanne, Switzerland (2022)

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

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

## AWARDS

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- **Chateaubriand Fellowship:** Awarded a prestigious fellowship by the Embassy of France on the United States to lead a joint research project between Université Paris-Saclay and Rutgers University that resulted in 5 peer-reviewed publications.
- **Dean Dissertation Fellowship:** Awarded for outstanding research contributions in applied physics.
- **ICIQ Summer Fellowship:** Top 1.4% among 1,000+ applicants for a prestigious research program in one of Spain's leading chemical institutions.
- **IFIMAC Grant:** Awarded a full-tuition M.Sc. scholarship and living stipend by the Institute of Condensed Matter Physics.