EVARISTO VILLASECO

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EDUCATION

Ph.D. in Theoretical 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

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

- **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.