Maria A. Castellanos

mariacm_12@hotmail.com +1 (754) 232 6562 New York, NY mariacastellanos1 mariacm12

Education

Ph.D. in Chemistry **Sept. 2018 - Nov. 2023**
Massachusetts Institute of Technology (GPA 4.7/5.0)
Advisor: Prof. Adam P. Willard.
Thesis: Theoretical Design of Molecular Nanostructures for Exciton Control.

Bsc. in Chemistry **Sept. 2012 - Aug. 2017**
Universidad Icesi, Cali, Colombia. *cum laude* (GPA 4.44/5.0)
Graduated first in the class. **Advisor:** Prof. Carlos A. Arango.
Thesis: Classical study of H + H interactions inside a Xe one-dimension cluster.

Experience

Postdoctoral Research Fellow **Jan. 2024 - Present**
Computational & Systems Biology, Sloan Kettering Institute, New York, NY
- Contributing to an open-science drug discovery pipeline, the *AI-driven Structure-enabled Antiviral Platform* (ASAP), aimed to accelerate structure-based drug discovery for wider access to pandemic therapeutics.
- Developing open-source computational chemistry software for testing the efficacy of potential anti-viral therapeutics in a set of identified relevant targets, such as variants of SARS-CoV-2.

Graduate Research Assistant **Jan. 2019 - Jan. 2024**
Department of Chemistry, MIT, Cambridge, MA
- Developed mathematical models and computational software to investigate and control the excited state properties of organic molecular systems, with applications in solar cell technology, and quantum information.
- Led the computational efforts in a multidisciplinary team of 7 graduate students and postdocs from experimental and theory groups at MIT, in designing programmable DNA scaffolds for organic devices.
- Developed a Python workflow for high-throughput screening of molecules attached to DNA nanostructures, automating force field development, molecular dynamics, quantum chemistry, and machine learning steps.
- Received comprehensive training in Python software best practices (*e.g.,* Git version control, unit tests, docstrings, package distribution) through the MolSSI Fellowship program.

Quantum Applications Intern **June - Aug. 2021 & June - Aug. 2022**
IBM Research, San Jose, CA
- Enhanced Python software to optimize the functionality of quantum computers in chemical applications.
- Utilized Q-Chem software to collect and analyze data on small molecule properties, presenting findings to diverse audiences of software engineers, physicists, and chemists.
- Initiated and conducted a research project utilizing quantum embedding techniques to calculate properties of large molecules, including electrostatic potential and force field partial charges.

Research Intern **Jan. 2017 - Apr. 2018**
Department of Chemistry, Universidad Icesi, Cali, Colombia
- Upgraded and improved genetic algorithms software in C++ for quantum optics applications.
- Developed a mathematical model to analyze the energy landscape of ultracold atoms.
- Trained and supervised two undergraduate students completing their thesis project within the group.

Research Intern **June - Aug. 2016**
Department of Chemistry, University of Rochester, Rochester, NY
- Upgraded and developed FORTRAN 90 software for studying Singlet Fission, a photophysical process that enhances solar cell efficiency, using a path-integral approach.

Research interests

- Molecular simulations for organic materials and biological applications.
- Machine learning applied to molecular modeling and simulations.
- Excited state electronic structure and dynamics.

Teaching Experience

Graduate Teaching Assistant **Sept. 2018 - May 2019**

Department of Chemistry, MIT, Cambridge, MA

Laboratory Chemistry & Principles of Chemical Science: Prepared lab sessions and recitations, graded reports and exams, and guided groups of 5-10 undergraduate students.

Laboratory Teaching Assistant **Aug. 2017 - June 2018**

Department of Chemistry, Universidad Icesi, Cali, Colombia

Laboratory Physical Chemistry: Trained groups of 15-20 students in laboratory practices for the introductory Physical Chemistry course. Prepared recitations and graded reports and exams.

Academic Projects

Publications

- **Castellanos M. A.** and Willard A. P. Controlling exciton dynamics with complex-valued coupling: A theoretical model study (*In preparation*).
- Gorman J.*, Hart S.*, John T, **Castellanos M. A.**, ..., Willard A. P., Schlau-Cohen G. and Bathe M. Nanoscale optimization of excitonic states using DNA origami. (submitted to *Chem*).
- **Castellanos M. A.**, Motta M. and Rice J. E. Quantum computation of $\pi \rightarrow \pi^*$ and $n \rightarrow \pi^*$ excited states of aromatic heterocycles. *Mol. Phys.* **2023**, *e2282736*.
- Hart S.*, Banal J.*, **Castellanos M. A.***, ..., Willard A., Bathe M. and Schlau-Cohen G. Activating charge-transfer state formation in strongly-coupled dimers using DNA scaffolds. *Chem. Sci.* **2022**, *13*, 13020-13031.
- **Castellanos M. A.** and Willard A. P. Designing excitonic circuits for the Deutsch–Jozsa algorithm: mitigating fidelity loss by merging gate operations. *Phys. Chem. Chem. Phys.* **2021**, *23*, 15196-15208.
- **Castellanos M. A.***, Dodin A.* and Willard, A. P. On the Design of Molecular Excitonic Circuits for Quantum Computing: The Universal Quantum Gates. *Phys. Chem. Chem. Phys.* **2020**, *22*, 3048-3057.
- Guerrero R. D, **Castellanos M. A.** and Arango C. A. Heuristic optimization of analytic laser pulses for vibrational stabilization of ultracold KRb. *J. Chem. Phys.* **2018**, *149*, 244110.
- **Castellanos M. A.** and Huo P. Enhancing Singlet Fission Dynamics by Suppressing Destructive Interference between Charge-Transfer Pathways. *J. Phys. Chem. Lett.* **2017**, *8* (11), pp 2480 – 2488.

(*) indicates equal contribution.

Ongoing Projects

Development of a Python package for high-throughput screening of properties of organic networks

- Designing a multi-step workflow incorporating classical molecular simulations, quantum chemistry calculations, and machine learning methods to investigate chromophores in DNA macromolecular scaffolding.
- Currently developing an open source project called `dyeScreen`, which is hosted on GitHub. The project utilizes various software packages including Amber, PySCF, Pandas, and MDAnalysis to enable efficient and accurate analysis of these molecular systems.
- Clustering and PCA methods will be employed to optimize the feature space of molecular geometries associating DNA scaffolding patterns with electronic structure properties, which could later be used to train a neural network.

Unsupervised machine learning models in exciton ensembles

- Training a Variational Autoencoder to learn the statistical properties of simple quantum mechanical systems and mitigate statistical noise.
- Exploiting the latent space dimensionality reduction of VAEs to gain insight on system-bath interactions of condensed-phase molecular systems.

Selected Academic Events

- **Castellanos M. A.** and Willard A. P. (Sept. 2023). Integrating Molecular Dynamics and Excited-State Quantum Mechanics for High-Throughput Screening of Molecules in Macromolecular Scaffolding. *MDAnalysis User Group Meeting (UGM) 2023*. University of Lisbon, Portugal. **(Oral presentation)**.
- **Castellanos M. A.**, Willard A. P. (March 2023). Imaginary excitonic coupling: Towards directional exciton flux in org. semiconductors. *American Chemical Society Spring Meeting*. Indianapolis, IN. **(Contributed talk)**.
- **Castellanos M. A.**, Hart S., Banal J. and Willard A. P. (March 2022). Steering dark state formation in molecular aggregates with DNA scaffolds: The interplay between Coulombic and charge transfer interactions. *American Physical Society March Meeting*. Chicago, Il. **(Contributed talk)**.
- **Castellanos M. A.** and Willard A. P. (October 2021). Designing quantum computers with molecular excitons: How can we mitigate the effect of the bath? *Greater Boston Area Statistical Mechanics Meeting*. Northeastern University. Boston, MA. **(Talk)**.
- **Castellanos M. A.**, Dodin A. and Willard A. P. (August 2019). Design of universal quantum gates using a molecular dye-based platform. *Penn Conference in Theoretical Chemistry.* University of Pennsylvania, Philadelphia. **(Poster)**.
- **Castellanos M. A.**, Dodin A. and Willard A. P. (August 2019). Design of universal quantum gates using a molecular dye-based platform. *Telluride School on Theoretical Chemistry.* Telluride Science Research Center. Telluride, Colorado. **(Poster)**.

Awards and Achievements

- Travel Grant Award to attend the **MDAnalysis UGM** conference 2023, granted by the organizing committee.
- Recipient of the 2022-2023 Molecular Sciences Software Institute (**MolSSI**) Fellowship.
- Amy Lin Shen Fellowship 2019, **MIT Department of Chemistry**.
- Scholarship for the Summer International Research Program 2016, **University of Rochester**.
- Academic excellence scholarship, **Universidad Icesi**.

Skills

Software:
Python (NumPy, SciPy, Pandas), C++, Wolfram Mathematica, Git, Linux, HPC

Computational Chemistry:
Electronic Structure (DFT, post-HF methods), Molecular Dynamics, Enhanced sampling, Genetic Algorithms, Quantum Embedding, *PySCF, Q-Chem, Psi4, Amber, MDAnalysis*

Machine Learning:
Deep Neural Networks (*VAEs, RNNs*), Data Visualization, Time Series, Classification, Clustering, *PyTorch, scikit-learn*

Languages: Spanish (Native), English (Fluent)

Collaboration, Commitment, Leadership, Verbal/Written Communication

Leadership Experience

Chemistry Alliance for Diversity and Inclusion **Sept. 2019 - Jan. 2021**
Department of Chemistry, MIT
Coordinated the organization of several events promoting inclusion in the Department. Designed, proposed and secured funding for a monthly discussion series: *Difficult conversations in the lab-space*.

MIT Colombian Association **Jan. 2019 - Present**
Led events promoting the Colombian culture at MIT. Administered the finances of the group.

Reviewer Activities

Journal of Chemical Theory and Computation.

References available upon request.