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# Sebastian Montillo Vega

## Statement

Computational chemist with 6+ years of experience developing high-performance simulation tools in quantum chemistry, molecular dynamics, and quantum dynamics. I build scalable computational workflows—integrating electronic-structure theory (Gaussian, Q-Chem, VASP), open-quantum-system modeling, and parallel Python/C++ implementations—to enable rigorous in-silico exploration of molecular and material systems. My work includes designing automated HPC workflows, applying ML frameworks (PyTorch, TensorFlow) for data analysis, and developing scientific software that accelerates simulation and discovery.

## Education

**University of Rochester** — Rochester, NY, USA
- Ph.D., Chemistry - Computational and Theoretical Chemistry. — **expected 2026**
- M.S., Chemistry. — 2022 - 2023

**University of Antioquia** — Medellín, Antioquia
- B.S., Chemistry, with Highest Honors. — 2014 - 2020

## Technical Skills

**Programming**
- Python (Numpy, SciPy, Numba), C++, Rust, Git, Linux, Pytorch, TensorFlow.

**Electronic-Structure & Molecular Dynamics**
- Gaussian, Q-Chem, VASP, LAMMPS, GROMACS.

**Quantum Simulation & Modeling**
- Open quantum systems, mixed quantum–classical dynamics, QuTiP, Qiskit.

**High-Performance & Parallel Computing**
- MPI, OpenMP, Slurm, HPC environments.

## Research and Technical Experience

**Graduate Research Fellow - Quantum Dynamics** — University of Rochester
- Developed new theoretical and computational approaches combining electronic-structure theory with QED Hamiltonians to study strongly correlated photon–matter states.
- Integrated TDDFT and many-electron response theory with cavity-QED models to analyze polarization effects, energy surfaces, and chemical reactivity.
- Developed high-performance quantum dynamics frameworks (HEOM, mixed quantum–classical) in Python and C++ to model light-matter interactions.
- Implemented MPI-parallelized and JIT-optimized propagation algorithms, reducing simulation runtimes by 50%+ and enabling studies of systems previously computationally intractable.
- Formulated new theoretical models that explain photon-induced reactivity trends in many-molecule systems and generated predictive insights used by experimental collaborators.
- Created scalable computational pipelines to explore strong light–matter coupling phenomena and benchmark theoretical predictions against experimental data.
- Analyzed high-dimensional electronic-structure datasets using automated Python workflows and HPC parallelization, improving the interpretability of photonic–molecular coupling effects.

**Undergraduate Research Assistant - Molecular Dynamics** — University of Antioquia
- Built Python packages to couple molecular-mechanics MD software (LAMMPS, GROMACS) with electronic-structure programs, enabling hybrid QM–MM simulations of complex biological environments.
- Developed analytical tools for large-scale spectroscopic and structural datasets to characterize molecular behavior in heterogeneous media using electronic structure methods such as Gaussian and VASP.
- Performed electronic-structure (VASP) and molecular dynamics (GROMACS) for materials modeling of oxide catalysts to understand reaction energetics and hydrogen-production pathways.

## Publications

**Theoretical Insights into the Resonant Suppression Effect in Vibrational Polariton Chemistry**
- Developed analytical models to explain cavity-modified chemical reactivity, validated through numerically exact quantum-dynamical simulations.
- **S. M. Vega**, W. Ying, and P. Huo.
- J. Am. Chem. Soc. 2025, 147 (23), 19727–19737.

**Polarized Fock States and the Dynamical Casimir Effect in Molecular Cavity Quantum Electrodynamics**
- Created theoretical frameworks that significantly reduced the computational cost of simulating light–matter interaction systems.
- A. Mandal, **S. M. Vega**, and P. Huo.
- J. Phys. Chem. Lett. 2020, 11 (21), 9215–9223.

**Evolution of Bonding during the Insertion of Anionic Ibuprofen into Model Cell Membranes**
- Implemented Python libraries to integrate classical molecular-dynamics simulations with electronic-structure programs to study drug absorption in lipid bilayers.
- N. Rojas-Valencia, S. Gómez, **S. M. Vega**, M. Manrique-Moreno, C. Cappelli, C. Hadad, and A. Restrepo.
- J. Phys. Chem. B 2020, 124 (1), 79–90.

**Infrared Plasmon Driven Acceleration of Photolysis Reaction**
- Developed theoretical models to explain chemical reactivity changes observed by experimental collaborators in plasmonic cavity systems.
- W. J. Chang, L. Carr, **S. M. Vega**, P. Huo, and D. J. Milliron.
- ChemRxiv

## Leadership and Outreach

**Diversity Equity and Inclusion Committee** University of Rochester
- Leader of the Transition to Rochester Advisory Committee, supporting international graduate students in adapting to life and academics in the Rochester area.

**Association of Latin American students (ALAS) - Vice President** University of Rochester
- Vice President of the Latin American Students Association, supporting community building and connection Latin American graduate students at the University of Rochester.

**Research Mentor** University of Rochester
- Mentored six undergraduate and graduate researchers in numerical modeling and software development for quantum and classical dynamics simulations, including Git-based collaborative workflows.

## Posters And Oral Presentations

Strong Coupling with Organic Molecules Conference (SCOM5) – **Poster**, 2025. *SDU, Denmark*
- Theoretical Insights into the Resonant Suppression Effect in Vibrational Polariton Chemistry.
- **S. M. Vega**, W. Ying, and P. Huo.

American Conference on Theoretical Chemistry (ACTC) – **Poster**, 2024. *University of South Carolina, USA*
- Theory of Resonant Suppression in Vibrational Polariton Chemistry.
- **S. M. Vega**, W. Ying, and P. Huo.