Alejandro Blanco-Gonzalez /alejandro-blanco-gonzalez, ablanco@attmosdiscovery.gmail.com

Research Experience

- **ATTMOS Inc. (Startup)| East Lansing, MI.**

  - **Research Scientist** 2024-present

  - **Research Consultant** 2024 (10 mos)
    - Designing, implementing, testing, and optimizing software components for the Automated Force Field Developer and Optimizer (AFFDO) platform. AFFDO is an advanced tool that rapidly generates refined force fields for accurate protein-ligand interaction analysis, aiming to streamline drug development by reducing time and costs while increasing precision.
    - Research interest: structure-based drug discovery (SBDD) methods, free energy perturbation (FEP), thermodynamic Integration (TI), molecular mechanics (MM) force fields development, molecular dynamics, high-throughput *ab initio* calculations, and software engineering.

- **Center for Photochemical Sciences, Bowling Green State University (BGSU) | Bowling Green, OH**

  - **Graduate Research/Teaching Assistant** 2018-2023
    - Research interests: semi-classical molecular dynamics, QM/MM methods, photoisomerization mechanism of molecular switches and motors, computational photochemistry, and photobiology.
    - Developed and automated scripts using Bash/Python for streamlining data processing, workflow automation, and enhancing the usability of QM/MM protocols.
    - Taught General Chemistry (labs and recitations).

- **Joint Institute for Nuclear Research (JINR), Flerov Laboratory of Nuclear Reactions (FLNR) | Dubna, Russia.**

  - **International Student Practices (Field of Research)** 2016
    - Research interests: synthesis and mass determination of super-heavy elements (112 and 114), mass spectroscopy, and nuclear reactions.

- **Higher Institute of Applied Sciences and Technologies (InSTEC), University of Havana (UH) | Havana, Cuba.**

  - **Instructor of Physical Chemistry and Research Assistant** 2015-2017
    - Teaching Quantum Chemistry, Nuclear Chemistry, and Radiochemistry (lectures).
    - Co-supervisor of research projects for undergraduate students pursuing a bachelor's degree in Radiochemistry.
    - M.S. research project: molecular modeling (DFT), the development of radiopharmaceuticals, physical chemistry, drug stability, and degradation studies.

- **Undergraduate Research/Teaching Assistant** 2013 - 2015
    - B.S. research project: molecular modeling (DFT), physical chemistry, radiochemistry techniques, and chemistry of radioactive elements.
    - Teaching Inorganic Chemistry and Physical Chemistry (labs).

❖ **Center for Drug Research and Development (CIDEM) | Havana, Cuba.**

- **Undergraduate Research Assistant** 2012-2013
    - Research interests: solvent extraction, organic chemistry, analytical and ultrasound techniques.

Education

Ph.D. Photochemical Sciences 2018 - 2023
Center for Photochemical Sciences, Bowling Green State University (BGSU) | Bowling Green, OH

M.S. Chemistry 2022 - 2023
Center for Photochemical Sciences, Bowling Green State University (BGSU) | Bowling Green, OH

M.S. Radiochemical Sciences, 2015 - 2017
Higher Institute of Applied Sciences and Technologies (InSTEC), University of Havana (UH) | Havana, Cuba.

B.S. Radiochemistry (summa cum laude), 2010 - 2015
Higher Institute of Applied Sciences and Technologies (InSTEC), University of Havana (UH) | *Havana, Cuba.*

Awards and Scholarship

- 3rd place in Oral Presentations at the Ohio Photochemical Society (OoPS) Meeting. July 2022, Bowling Green, OH, US. 2022
- National Union of Students award for outstanding teaching labor in Quantum Chemistry subject at the Higher Institute of Applied Sciences and Technologies (InSTEC), University of Havana (UH), Cuba. 2016
- Cuban Agency of Nuclear Energy and Advanced Technologies (AENTA) Scholarship for participation in the International Student Practices at the Joint Institute for Nuclear Research (JINR), Dubna, Russia. 2016
- Best poster at the II Symposium of Molecular Images Cuba-Japan 2016. Havana, Cuba. 2016
- Cuban Agency of Nuclear Energy and Advanced Technologies (AENTA) Award for Best Graduate of Nuclear Careers. Havana, Cuba. 2015
- Multiple awards at the Scientific Student Competition InSTEC-UH, Havana, Cuba. These accolades include the Special Prize "Grand Prize InSTEC" for the best work of the event, the Prize "Bigger Scientific Contribution" of the event, and the 1st Prize in the Radiochemistry section. 2015
- 3rd Prize in the Radiochemistry section at the Scientific Student Competition InSTEC-UH, Havana, Cuba. 2014
- 2nd Prize in the Didactic of Teaching section at the Scientific Student Competition of InSTEC-UH, Havana, Cuba. 2013

- 2nd Prize in the Teaching of Sciences section at the Scientific Student Competition of InSTEC-UH, Havana, Cuba. 2011

PUBLICATIONS

- Blanco-Gonzalez, A., Kaliakin, D., Filatov(Gulak), M., Paolino, M., Leonard, J., Olivucci, M. (2025). *"Population Dynamics of a Photon-Only Molecular Motor Shows That Mode Synchronization and Transient Binding Determine the Rotary Quantum Efficiency"* J. Chem. Theory Comput. 2025, XXXX, XXX, XXX-XXX 2025
- Blanco-Gonzalez A, Betancourt W, Snyder R, Zhang S, Giese TJ, Goetz AW, et al. *"Automated Force Field Developer and Optimizer Platform: Torsion Reparameterization."* ChemRxiv. 2024 2024
- Blanco-Gonzalez, A., Manathunga, M., Yang, X., Olivucci M. (2024). *"Comparative quantum-classical dynamics of natural and synthetic molecular rotors show how vibrational synchronization modulates the photoisomerization quantum efficiency."* Nat Commun 15, 3499. 2024
- Simachew Bezabih, M., S. Kaliakin, D., Blanco-González, A., Barneschi, L., N. Tarnovsky, A., & Olivucci, M. (2023). *"Comparative Study of Uracil Excited-State Photophysics in Water and Acetonitrile via RMS-CASPT2-Driven Quantum-Classical Trajectories"*. The Journal of Physical Chemistry B, 0(0). 2023
- Manni, G. L., Galván, I. Fdez., Alavi, A., Aleotti, F., Aquilante, F., Autschbach, J., Avagliano, D., Baiardi, A., Bao, J. J., Battaglia, S., Birnoschi, L., Blanco-González, A., Bokarev, S. I., Broer, R., Cacciari, R., Calio, P. B., Carlson, R. K., Couto, R. C., Cerdán, L., … Lindh, R. (2023). *"The OpenMolcas Web: A Community-Driven Approach to Advancing Computational Chemistry."* Journal of Chemical Theory and Computation, 19 (20), 6933-6991. 2022
- Barneschi, L., Marsili, E., Pedraza-González, L., Padula, D., de Vico, L., Kaliakin, D., Blanco-González, A., Ferré, N., Huix-Rotllant, M., Filatov, M., Olivucci, M. (2022). *"On the fluorescence enhancement of arch neuronal optogenetic reporters."* Nature Communications, 13 (1), 6432. 2022
- Filatov(Gulak), M., Paolino, M., Pierron, R., Cappelli, A., Giorgi, G., Léonard, J., Huix-Rotllant, M., Ferré, N., Yang, X., Kaliakin, D., Blanco-González, A., Olivucci, M. (2022). *"Towards the engineering of a photon-only two-stroke rotary molecular motor."* Nature Communications, 13 (1), 6433. 2022
- Chatterjee, G.,***** Jha, A.,***** Blanco-Gonzalez, A.,***** Tiwari, V., Manathunga, M., Duan, H. G., Tellkamp, F., Prokhorenko, V. I., Ferré, N., Dasgupta, J., Olivucci, M., Miller, R. J. D. (2022). *"Torsionally broken symmetry assists infrared excitation of biomimetic charge-coupled nuclear motions in the electronic ground state."* Chemical Science. 13 (32), 9392–9400. *****Authors contributed equally and are considered co-first authors.
- Hernández-Valdés, D., Blanco-González, A., García-Fleitas, A., Rodríguez-Riera, Z., Meola, G., Alberto, R., & Jáuregui-Haza, U. (2017) *"Insight into the structure and stability of Tc and Re DMSA complexes: A computational study."* Journal of Molecular Graphics and Modelling, 71 167–175. 2017
- Jáuregui, U.; Blanco, A.; Hernández, D.; García, A.; Rodríguez, Z.; (2016). *"Actualidad y retos de la química de los complejos ^{99m}Tc,$^{186/188}$Re-DMSA."* ALASBIMN Journal, ISSN: 0717 - 4055. 2016
- Rodríguez-Riera Z, Robaina-Mesa M, Jáuregui-Haza U, Blanco-González A, Rodríguez-Chanfrau J. (2014) *"Empleo de la radiación ultrasónica para la extracción de compuestos bioactivos provenientes de fuentes naturales. Estado actual y perspectivas."* Revista CENIC Ciencias Químicas, Vol. 45, pp. 139-147. 2014

Unpublished Works

- Obloy, L.,***** Valloi, L. K.,***** Blanco-Gonzalez, A.,***** Olivucci, M., Tarnovsky, A., Sivaguru, J. (2025). *"Deciphering Novel Photoreactivity of β-Enaminones"* Manuscript under review. *****Authors contributed equally and are considered co-first authors. 2025

Contributed Talks

- Ohio Photochemical Society Meeting (OoPS) Meeting. July 2022, Bowling Green, OH, US. "Torsionally broken symmetry assists infrared excitation of biomimetic charge-coupled nuclear motions in the electronic ground state." (Third place Oral Presentation) 2022
- 52nd Midwest Theoretical Chemistry Conference (MWTCC). June 2022, Columbus, OH, US. "Torsionally broken symmetry assists infrared excitation of biomimetic charge-coupled nuclear motions in the electronic ground state." 2022
- ACS Spring Meetings, 2022. The Synergy of Theory and Experiment: A Symposium in Honor of Prof. John F. Stanton. March 2022, San Diego, CA, US. "Vibrationally-induced ground-state charge transfer in a donor-bridge-acceptor in solution: A multi-reference quantum chemical population dynamics study." 2022
- 3rd International Congress on Research, Development, and Technological Innovation in the BioPharmaceutical Industry (IDIFARMA 2016). Havana, Cuba. December 2016. "Quality evaluation of DMSA, raw material for producing radiopharmaceuticals." 2016
- 10th International Congress of Higher Education "University 2016", X Workshop InSTEC. Havana, Cuba, March 2015. "Theoretical study of Tc and Re-DMSA complexes used in Radiopharmacy." 2015
- 9th International Congress of Higher Education "University 2016", IX Workshop InSTEC. Havana, Cuba, April 2013. "Ultrasound-assisted extraction of bioactive compounds: From research to the teaching laboratory." 2013

Contributed Posters

- 11th Seminars of Advanced Studies on Molecular Design and Bioinformatics (SEADIM). Varadero, July 2017, Cuba. "Theoretical study of DMSA degradation reaction" 2017
- V International Seminar of Center of Isotopes (CENTIS). Havana, Cuba. February 2016. "Insight into the structures and stabilities of Tc and Re DMSA complexes: A computational study." 2016
- II Symposium of Molecular Images Cuba-Japan. Havana, Cuba. January 2016. "Potentials of computational modeling to design of radiopharmaceutical" (Award to Best Poster). 2016
- 9th Congress of Chemical Sciences, Technology, and Innovation (Quimicuba 2015). Havana, Cuba. October 2015. "A Theoretical Study of the Complexes Technetium and Rhenium DMSA" 2015
- 10th Seminars of Advanced Studies on Molecular Design and Bioinformatics (SEADIM). Havana, Cuba. June 2015. "DMSA and its complexes with Technetium and Rhenium: a computational study" 2015
- XV Workshop on Nuclear Physics (XV WONP) and IX International Symposium on Nuclear and Related Techniques. (IX NURT). Havana, Cuba. February 2015. "A theoretical NMR study of rhenium and technetium DMSA complex" 2015

Skills

- Proficient in utilizing various quantum chemistry and molecular dynamics packages such as GAUSSIAN, [Open]MOLCAS, GROMACS, TINKER, QUICK, AMBER and visualization software.
- Python (libraries like NumPy, SciPy, Pandas, Matplotlib, etc), Bash Scripting,
- SQL (toolkit like SQLAlchemy), Sphinx, HTML, Streamlit
- UNIX/Linux systems.

Languages

Spanish - Native language.
English - Professional working proficiency.