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Education

2008 - 2012 **Ph.D. in Physics**, Universidade de São Paulo (USP), São Paulo, Brazil.
Title: "Photophysics and dynamical properties of molecular systems".
Advisor: Prof. Sylvio Canuto

2006 - 2008 **M.Sc. in Physics**, Higher Institute of Technologies and Applied Sciences (INSTEC), Havana, Cuba.
Advisor: Prof. Maikel Y Ballester

2000 - 2005 **B.S. (Summa cum Laude) in Nuclear Physics**, Higher Institute of Technologies and Applied Sciences (INSTEC), Havana, Cuba.

Professional Experience

2017 – Present Postdoctoral Research. Georgia State University, Atlanta, USA.
Advisor: Prof. Samer Gozem

2015 – 2017 Postdoctoral Research. Institut de Physique et Chimie des Materiaux de Strasbourg (IPCMS), Strasbourg, France.
Advisors: Prof. Massimo Olivucci, Prof. Stefan Haacke

2012 – 2015 Postdoctoral Research. University of São Paulo, São Paulo, Brazil and Bowling Green State University, Bowling Green, USA.
Advisors: Prof. Sylvio Canuto, Prof. Massimo Olivucci

Publications

1. Electronic Spectra of Flavin in Different Redox and Protonation States: A Computational Perspective on the Effect of the Electrostatic Environment.

M. P. Kabir, Y. Orozco-Gonzalez, S. Gozem. ***Physical Chemistry Chemical Physics*** 21, 16526-16537 (2019).

2. Electrostatic Spectral Tuning Maps for Biological Chromophores.
   Y. Orozco-Gonzalez, M. P. Kabir, S. Gozem. ***The Journal of Physical Chemistry B*** 123 (23), 4813-4824 (2019).

3. Fluorescence Properties of Flavin Semiquinone Radicals in Nitronate Monooxygenase.
   D. Su, M. P. Kabir, Y. Orozco-Gonzalez, S. Gozem, G. Gadda. ***ChemBioChem*** 20 (13), 1646-1652 (2019).

4. Anabaena Sensory Rhodopsin: Effect of point mutations on PSBR photo-isomerization speed.
   D. Agathangelou, Y. Orozco-Gonzalez, M. C. Marin, J. Brazard, H. Kandori, K. Jung, J. Léonard, N. Ferré, M. Olivucci, S. Haacke. ***The European Physical Journal Conferences*** 205, 10004 (2019).

5. Fluorescence enhancement of a microbial rhodopsin via electronic reprogramming.
   M. C. Marín, D. Agathangelou, Y. Orozco-Gonzalez, A. Valentini, Y. Kato, R. Abe-Yoshizumi, H. Kandori, A. Choi, K. Jung, S. Haacke, M. Olivucci. ***Journal of the American Chemical Society*** 141 (1), 262-271 (2018).

6. Effect of point mutations on the ultrafast photo-isomerization of Anabaena sensory rhodopsin. D. Agathangelou, Y. Orozco-Gonzalez, M. del Carmen Marín, P. P. Roy, J. Brazard, H. Kandori, K-H. Jung, J. Leonard, T. Buckup, N. Ferré, M. Olivucci, and S. Haacke. ***Faraday Discussions*** 207, 55-75 (2018).

7. Engineering the vibrational coherence of vision into a synthetic molecular device.
   M. Gueye, M. Manathunga, D. Agathangelou, Y. Orozco-Gonzalez, M. Paolino, S. Fusi, S. Haacke, M. Olivucci, J. Leonard. ***Nature Communications*** 9, 313 (2018).

8. An Average Solvent Electrostatic Configuration Protocol for QM/MM Free Energy Optimization: Implementation and Application to Rhodopsin Systems.
   Y. Orozco-Gonzalez, M. Manathunga, M. del Carmen Marín, D. Agathangelou, K-H. Jung, F. Melaccio, N. Ferré, S. Haacke, K. Coutinho, S. Canuto, M. Olivucci. ***Journal of Chemical Theory and Computation*** 13(12) 6391-6404 (2017).

9. Impact of Electronic State Mixing on the Photoisomerization Timescale of the Retinal Chromophore.
   M. Manathunga, X. Yang, Y. Orozco-Gonzalez, M. Olivucci. ***The Journal of Physical Chemistry Letters*** 8, 5222-5227 (2017).

10. Toward Automatic Rhodopsin Modeling as a Tool for High-Throughput Computational Photobiology.
    F. Melaccio, M. del Carmen Marin, A. Valentini, F. Montisci, S. Rinaldi, M. Cherubini, M. Stenrup, Y. Orozco-Gonzalez, N. Ferre, H. Ling Luk, and M. Olivucci. ***Journal of Chemical Theory and Computation*** 12 (12), 6020–6034 (2016).

11. Solvent Effects on the Dynamic Polarizability and Raman Response of Molecule–Metal Oxide Hybrid Clusters.
    Y. Orozco-Gonzalez, P. Tarakeshwar, S. Canuto, V. Mujica. ***ChemPhysChem*** 2590-2595 (2016).

12. Solvent effect on the Stokes shift and on the nonradiative decay of the daidzein molecular system.
    Y. Orozco-Gonzalez, C. Bistafa, K. Coutinho, S. Canuto. ***The Journal of Physical Chemistry*** A 117, 4404 (2013).

13. Theoretical study of the absorption and nonradiative deactivation of 1-Nitronaphthalene in the low-lying singlet and triplet excited states including methanol and ethanol solvent effects.
    Y. Orozco-Gonzalez, K. Coutinho, J. Peon, S. Canuto. ***The Journal of Chemical Physics*** 137, 054307 (2012).

14. CASPT2 study of the potential energy surface of the HSO2 system.
    J. D. Garrido, M. Y. Ballester, Y. Orozco-Gonzalez, S. Canuto. ***The Journal of Physical Chemistry*** A 115, 1453 (2011).

15. Excited state electronic polarization and reappraisal of the n←pi* emission of acetone in water.
    Y. Orozco-Gonzalez, K. Coutinho, S. Canuto. ***Chemical Physics Letters*** 499, 108 (2010).

16. A quasiclassical trajectory study of the OH plus SO reaction: The role of rotational energy.
    M. Y. Ballester, Y. Orozco-Gonzalez, J. D. Garrido, H. F. Dos Santos. ***The Journal of Chemical Physics*** 132, 044310 (2010).

17. Toward a global double many body expansion potential energy surface of the $SO_3(^3A)$; quasi-classical trajectory study of the reaction $S(^3P)+O_3(^1A_1)$.
    Y. Orozco-Gonzalez, M. Y. Ballester, F. Jorge-Lazo. ***Cuban Journal of Physics*** 26 2B, 267 (2009).

Conferences

1. ***Scientific Computing Day.***
   Georgia State University, Atlanta, GA. USA, 2018.
   Poster presentation: Modeling the spectral properties of flavin cofactor in different environments by using hybrid quantum/classical approaches.

2. ***Atlanta Mini Symposium on Theoretical and Computational Chemistry***.

Emory University, Atlanta, GA, USA. 2018.
Poster presentation: Average electrostatic approach for multi-configurational QM/MM.

3. ***Exited States Bridging Scales***.
   Marseille, France, November 7-10, 2016.
   Oral presentation: QM/MM Geometry Optimization of Chromophore-Protein complex using the ASEC Free Energy Gradient.

4. ***II Workshop on Biomolecular Theory-Experiment Interplay***. Maresias, Sao Paulo, Brazil. Aug 30 – Sep 03, 2015.
   Oral Presentation: Average Solvent Electrostatic Configuration and the free energy gradient method applied to the study of spectroscopic properties of proteins.

5. ***Third Workshop on Atomic and Molecular Pgysics***.
   Varadero, Cuba, June 29 - July 3, 2015
   Oral Presentation: Study of Spectroscopic properties of molecular systems embedded in complex environments considering the free energy surface.

6. ***Brazilian Physical Society Meeting (XXXVIII ENFMC).***
   Foz do Iguaçu, Parana, Brazil. May 24 – 28, 2015.
   Oral Presentation: Free energy geometry optimization of molecular systems embedded in complex environments.

7. ***XXVI IUPAP Conference on Computational Physics, CCP2014***.
   Boston University, Boston, Massachusetts, USA. Aug 11-14, 2014.
   Poster Presentation: Implementation of the Free Energy Gradient to the Geometry Optimization of Molecular Systems in Complex Environments.

8. ***7th International Meeting on Photodynamics and Related Aspects***.
   Maresias, São Paulo, Brazil. October 14-20, 2012.
   Oral Presentation: Photophysics of the 1-Nitronaphthalene molecular system.

9. ***Ninth Trienal Congress of the World Association of Theoretical and Computational Chemistry (WATOC).***
   Santiago de Compostela, Spain. June 17-22, 2011.
   Poster Presentation: Theoretical study of photophysical phenomena in 1-nitronaphthalene molecular system including methanol and ethanol solvent effects.

10. ***Sixth International Meeting on Photodynamics.***
    Havana, Cuba. February 1-5, 2010.
    Poster Presentation (1): The emission spectrum of acetone in water including the polarization of the excited state.
    Poster Presentation (2): A quasi-classical trajectory study of the OH+SO reaction: The role of rotational energy.

11. ***XXXIII Encontro Nacional de Física da Matéria Condensada.***

Águas de Lindóia, Brazil. May 10-14, 2010.
Poster Presentation: Theoretical study of the Intersystem crossing in 1-nitronaphtalene molecular system and the effect of the methanol solvent.

12. ***XV Simpósio brasileiro de química teórica (SBQT).***
Poços de caldas, Brazil. October 18-21, 2009.
Poster Presentation: Electronic transitions of the acetone in water.

13. ***Fifth international meeting on photodynamics.***
Havana, Cuba. February 4-8, 2008.
Poster Presentation: Quasi-classical trajectory study of the reaction $S(^3P)+O_3(^1A_1)$ by using the DMBE $2+3+4_{ele}$ potential energy surface of $SO_3(^3A)$.

14. ***III Convención Científica Internacional de la Universidad de Matanzas (CIUM).***
Varadero, Cuba. June 13-15, 2007.
Oral Presentation: Toward a double many-body expansion potential energy surface for the triplet electronic state of SO_3.

15. ***XXXIII Congreso de Químicos Teóricos de Expresión Latina, (QUITEL 33).***
Havana, Cuba. September 17-21, 2007.
Poster Presentation: Modeling a four-body electrostatic energy term for a double many-body expansion potential energy surface of $SO_3(^3A)$.

Developed codes

- ***APEC-FEG*** (link): A unique QM/MM method interfaced with Gromacs, Molcas, and Tinker for performing Quantum Mechanics calculations in a superposition of protein configurations.
Languages used: Python, Bash, Fortran
Main programmer

- ***ARM*** (link): An efficient protocol for automatic construction of QM/MM models
Languages used: Bash
Contributing programmer

- ***ESTM generator*** (link): A series of Python/Bash scripts to generate “electrostatic spectral tuning maps" from quantum mechanical calculations.
Languages used: Python, Bash
Main programmer

- ***ESTM Web Site*** (In development): A website to submit and visualize ESTM jobs.
Languages used: JavaScripting, PHP, Python, Bash
Main programmer

- ***Machine Learning*** (Github private repository): Random Forest and Support Vector Machine codes developed to recognize pattern in large data sets.
  Languages used: Python (Scikit-learn).
  Main programmer

- ***Deep Learning***: (Github private repository): Long Short-Term Memory (LSTM) RNN combined with a 1D Convolutional kernel to predict trend and recognize patterns in large data sets.
  Languages used: Python (KERAS running on top of TensorFlow) and trained on the GPU resources of the AWS cloud.
  Main programmer

Mentoring and Team work

- Worked closely with a very diverse team of people.
- Mentored several graduate students to develop their knowledge in science, programming and computational skills.
- Held "Coding club" sessions at Georgia State University where I trained a group of ~10 students in using Python, Bash scripting and Machine Learning.

Languages

- English: Full Professional Working Proficiency.
- Portuguese: Full Professional Working Proficiency.
- Spanish: Native proficiency.