Yoelvis Orozco González

Curriculum Vitae (09/2017)

Personal Information

Full name: Yoelvis OROZCO-GONZALEZ, Ph.D.

Current Professional Positions:
Institut de Physique et Chimie des Materiaux de Strasbourg (IPCMS)
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Work history

2015 - 2017 Post-doc with Profs. Stefan Haacke, Jérémie Leonard and Massimo Olivucci at Institut de Physique et Chimie des Materiaux de Strasbourg (IPCMS), Strasbourg, France.

2014-2015 Post-doc with Prof. Sylvio Canuto
Universidade de São Paulo (USP), São Paulo, Brazil.

2013 – 2014 Post-doc with Prof. Massimo Olivucci and Prof. Sylvio Canuto Bowling Green State University, Bowling Green, Ohio, USA and Universidade de São Paulo (USP), São Paulo, Brazil.

2012 - 2013 Post-doc with Prof. Sylvio Canuto
Universidade de São Paulo (USP), São Paulo, Brazil.

Education

2008 - 2012 Ph.D. in Physics
Universidade de São Paulo (USP), São Paulo, Brasil
Title: “Photophysics and dynamical properties of molecular systems”
Supervisor: Dr. Sylvio Roberto Accioly Canuto.

2006 - 2008 M.Sc. in Physics
Instituto Superior de Tecnologias y Ciencias Aplicadas (INSTEC), Havana, Cuba
Title: “Global potential energy surface for the $SO_3(^3A)$ molecular system”
Supervisor: Dr. Maikel Yusat Ballester Furones.

2000 - 2005 B.S. (*Summa cum Laude*) in Nuclear Physics
Instituto Superior de Tecnologias y Ciencias Aplicadas (INSTEC), Havana, Cuba
Title: "Chemical physics model in the interaction of the catechin with the elastase and renin proteins".
Supervisor: Dra. Edelsis Codorniu Hernández

Awards

2008 Sello Forjadores del Futuro. Ministerio de Ciencia Tecnologia e Medio Ambiente, Habana Cuba.
(Builders of the Future. Ministry of Science, Technology and Environment, Havana, Cuba).

Research Interests

- Atomic and molecular physics
- Quantum Mechanics
- Excited electronic states
- Molecular dynamics
- Solvent effect
- Free energy calculations

Publications

- New insights on the absorption and fluorescent emission of Prodan. C. Vequi-Suplicy, Y. Orozco-Gonzalez, M. Teresa Lamy, S. Canuto, K. Coutinho. ***In process for submission***.
- Effect of point mutations on the ultrafast photo-isomerization dynamics in 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. ***Submitted to Faraday Discussions on Sep 27, 2017***.
- Engineering the vibrational coherence of vision into a synthetic molecular device. M. Gueye, M. Manathunga, Y. Orozco-Gonzalez, M. Paolino, S. Fusi, S. Haacke, M. Olivucci, J. Leonard. ***Submitted to Nature Communications on Jul 11, 2017***.
- QM/MM Free Energy Optimization of Light-Responsive Proteins via the ASEC-FEG protocol. 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. ***Submitted to J. Chem. Theory Comput. on Aug 22, 2017***.

- Impact of Electronic State Mixing on the Photoisomerization Timescale of the Retinal Chromophore. M. Manathunga, X. Yang, Y. Orozco-Gonzalez, M. Olivucci. ***Accepted for publication in J. Phys. Chem. Lett. on Sep 13, 2017****.*
- Automatic Rhodopsin Modeling as a Prospective Tool for High-throughput 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. ***J. Chem. Theory Comput.*** 12 (12), 6020–6034 (2016).
- Solvent Effects on the Dynamic Polarizability and Raman Response of Molecule–Metal Oxide Hybrid Clusters. Y. Orozco-Gonzalez, P. Tarakeshwar, S. Canuto, V. Mujica. ***Chem.Phys.Chem.*** DOI: 10.1002/cphc.201600164.
- 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. ***J. Phys. Chem. A*** 117, 4404 (2013).
- 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. ***J. Chem. Phys.*** 137, 054307 (2012).
- CASPT2 study of the potential energy surface of the HSO_2 system. J. D. Garrido, M. Y. Ballester, Y. Orozco-Gonzalez, S. Canuto. ***J. Phys. Chem. A*** 115, 1453 (2011).
- 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. ***J. Chem. Phys.*** 132, 044310 (2010).
- Excited state electronic polarization and reappraisal of the n←pi* emission of acetone in water. Y. Orozco-Gonzalez, K. Coutinho, S. Canuto. ***Chem. Phys. Lett.*** 499, 108 (2010).
- 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. ***Rev. Cub. Fis.*** 26 2B, 267 (2009).

Participation in Scientific Events

- 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.

- 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.
- 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.
- Brasilian Physical Society Meeting 2015 (XXXVIII ENFMC).

  Foz do Iguaçu, Parana, Brazil. May 24 – 28, 2015.

  Oral Presentation: Free energy geometry optimization of molecular systems embedded in complex environments.
- 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.
- Ninth Trienal Congress of the World Association of Theoretical and Computational Chemistry (WATOC-2011).

  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.
- 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.
- 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.
- XV Simpósio brasileiro de química teórica (SBQT).

  Poços de caldas, Brazil. October 18-21, 2009.

  Poster Presentation: Electronic transitions of the acetone in water.
- 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 $SO_3(^3A)$.

- 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.
- 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 $SO_3(^3A)$.

Workshops and schools

2010	6th MOLCAS Workshop Universidade de São Paulo (USP), São Paulo, Brazil August 09-13, 2010
2010	Monte Carlo and molecular Dynamics Universidade de Brasília (UNB), Brasília, Brazil July 18-21, 2010