Roberto Olivares-Amaya

CONTACT INFORMATION

Harvard University
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RESEARCH INTERESTS

Quantum Chemistry, Spectroscopy, Photovoltaics, Surface Enhanced Raman Scattering, Charge and Energy Transfer, Sustainability, Computational Chemistry, Cheminformatics, Graphics Processing Units.

EDUCATION

Harvard University, Cambridge, Massachusetts, USA

Ph. D. Candidate, Department of Chemistry and Chemical Biology,
2007 to present GPA: 3.6

- Preliminary thesis title: *Molecular Response in Nanoscale Environments*
- Advisor: Prof. Alán Aspuru-Guzik
- Area of Study: Chemical Physics

University of California, Berkeley, Berkeley, California, USA

Exchange Student Chemistry, 2005-2006 GPA: 4.0

National Autonomous University of Mexico, UNAM, Mexico City, Mexico

B.Sc., Chemistry, 2002-2006 GPA: 3.93

- *Gabino Barreda Medal*, with Honors in Chemistry

AWARDS AND SCHOLARSHIPS

Harvard University

- Center for International Development, Giorgio Ruffolo Doctoral Fellow in Sustainability Science, 2010-2011
- Harvard University Center for the Environment Graduate Consortium on Energy and Environment, 2009
- Graduate School of Arts and Sciences CONACYT-Fundación-Harvard University Graduate School of Arts and Sciences Fellowship, 2007

American Conference on Theoretical Chemistry

- Travel Fellowship, 2011

Department of Energy

- Materials for Energy Applications Travel Fellowship, 2011
- Molecular Quantum Mechanics Travel Fellowship, 2010

American Chemical Society

- Chemical Computing Group Research Excellence Award, 2010

National Science Foundation

- Materials Computation Center (UIUC) — NSF Travel Grant, TDDFT Prospects and Applications Workshop and School, 2008

Gordon Research Conference

- Carl Storm International Diversity Fellowship Time-Dependent Density-Functional Theory, 2007

UNAM

- Gabino Barreda Medal Awarded to highest GPA student in each concentration, 2006
    - Best Student Poster, 40th Mexican Chemical Congress

Professional Experience

Harvard University, Cambridge, Massachusetts USA

Graduate Research Assistant, Chemical Physics *July 2007 to present*

- Research with Prof. Alan Aspuru-Guzik on the areas of theoretical chemistry, spectroscopy, cheminformatics and computational chemistry.
- Founding member of the IBM/Harvard Clean Energy Project. Began a distributed computing endeavor to study electronic properties of conjugated polymers to find more efficient organic solar cells.
- Develop Poisson-Schrödinger program to calculate molecular properties under complex electrostatic environments.
- Perform theoretical studies of surface enhanced Raman scattering (SERS) to understand the enhancement mechanism, and in particular, chemical enhancement.
- Accelerated quantum chemistry algorithms using graphics processing units.
- Mentor undergraduate students with their own research projects.

National Autonomous University of Mexico (UNAM) Mexico City, Mexico

Undergraduate Researcher *August 2006-July 2007*

- Research with Prof. Carlos Amador-Bedolla on the areas of theoretical chemistry and computational chemistry. Modeled the exchange-correlation hole in DFT for helium and lithium.

University of California-Berkeley Berkeley, California, USA

Undergraduate Researcher *January-July 2006*

- Research with Prof. William Lester on the areas of theoretical chemistry and computational chemistry. Computational improvement of a quantum Monte Carlo program.

Undergraduate Researcher *August-December 2005*

- Research with Prof. John Arnold on the areas of organometallic chemistry. Designed ligands for organometallic chemistry synthesis.

Teaching Experience

Harvard University, Cambridge, Massachusetts USA

Teaching Fellow, Physical Properties of Macromolecules *Jan. 2009 - June 2009*

Teaching Fellow, Statistical Thermodynamics *Jan. 2008 - June 2008*

Research Publications

Technical Articles

1. R. Olivares-Amaya, C. Amador-Bedolla, J. Hachmann, S. Atahan-Evrenk, R.S. Sánchez-Carrera, L. Vogt, A. Aspuru-Guzik *Accelerated computational discovery of high-performance materials for organic photovoltaics by means of cheminformatics*, *Submitted*

2. J. Hachmann, R. Olivares-Amaya, S. Atahan-Evrenk, C. Amador-Bedolla, R.S. Sánchez-Carrera, A. Gold-Parker, L. Vogt, A.M. Brockway, A. Aspuru-Guzik *The Harvard Clean Energy Project: Large-scale computational screening and design of organic photovoltaics on the World Community Grid*, *Submitted*

3. R. Olivares-Amaya, M. Stopa, X. Andrade, M.A. Watson and A. Aspuru-Guzik *Anion Stabilization in Electrostatic Environments*, J. Phys. Chem. Lett., **2011**, 2, 682-688.

4. D.G. Tempel, M.A. Watson, R. Olivares-Amaya and A. Aspuru-Guzik *Theory of Excitation Broadening using Time-Dependent Density Functional Theory for Open Quantum Systems*, J. Chem. Phys., **2011**, 134, 074116.

5. M.A. Watson, R. Olivares-Amaya, R.G. Edgar, and A. Aspuru-Guzik, *Accelerating correlated quantum chemistry calculations using graphical processing units*, Comput. Sci. Eng., **2010**, 12, pp. 40–51.

6. R. Olivares-Amaya*, M.A. Watson*, R.G. Edgar, L. Vogt, Y. Shao, and A. Aspuru-Guzik, *Accelerating correlated quantum chemistry calculations using graphical processing units and a mixed-precision matrix multiplication library (MGEMM)*, J. Chem. Theory and Comput., **2010**, 6, 135–144.

7. S. K. Saikin, R. Olivares-Amaya, D. Rappoport, M. Stopa, and A. Aspuru-Guzik, *On the chemical bonding effects in the Raman response: Benzenethiol adsorbed on silver clusters*, Phys. Chem. Chem. Phys. **2009**, 11, 9401–9411.

8. R. Olivares-Amaya, R. Salomon-Ferrer, W. A. Lester Jr., and C.Amador-Bedolla, *Creation of a GUI for Zori, a Quantum Monte Carlo program, using Rappture*, Comput. Sci. Eng., **2009**, 11, 41–47.

9. L.Vogt*, R. Olivares-Amaya*, S. Kermes, Y. Shao, C. Amador-Bedolla and A. Aspuru-Guzik *Accelerating resolution-of-the-identity second-order Moller-Plesset calculations using graphical processing units*, J. Phys. Chem. A **2008**, 112, 2049–2057.

In Preparation

10. R. Olivares-Amaya, D. Rappoport, Philip Muñoz, P. Peng, E. Mazur, A. Aspuru-Guzik *On mixed-metal surface-enhanced Raman scattering*

11. R. Olivares-Amaya, S. Atahan-Evrenk, J. Hachmann, C. Amador-Bedolla, A. Aspuru-Guzik *Generation of a molecular library for donor and acceptor organic-photovoltaic materials*

Relevant Presentations

Talks, Posters and Stays

1. *Chemical Effects in Surface-Enhanced Raman Scattering* Contributed Poster at the American Conference on Theoretical Chemsitry. Telluride, CO (July, 2011)

2. *Finding Organic Photovoltaic Materials One Screensaver at a Time*, Contributed Poster at USC-DOE Conference on Materials for Energy Applications: Experiment, Modeling and Simulations. Rancho Palos Verdes, CA (March, 2011)

3. *Creating reaction schemes to generate an arbitrary number of linked and conjugated polymers*, Contributed Talk at ACS Meeting 2010. Boston, MA (August, 2010)

4. *Benzene Anion Stabilization under a Complex Electrostatic Environment*, Contributed Poster at ACS Meeting 2010. Boston, MA (August, 2010)

5. *Anion Stabilization in Electrostatic Environments*, Contributed Poster at the 11th Sostrup Summer School: Quantum Chemistry and Molecular Properties. Sostrup, Denmark (July, 2010)

6. *Quantum Chemistry on Electrostatic Environments.* Invited Stay at the European Theoretical Spectroscopy Facility of San Sebastian, Spain (August 2009)

7. *Quantum Chemistry on Electrostatic Environments.* Contributed Poster at American Chemical Society Fall Meeting, Washington, D.C. (August, 2009)

8. *Surface-Enhanced Raman Scattering.* Contributed Poster at DARPA SERS Science and Technology Meeting, Minneapolis, MN (January, 2009)

9. *Renewable Energy and Free Software (In Spanish)* Invited Talk at CONSOL, Mexico City, Mexico (February, 2008)

10. *Accelerating Quantum Chemistry Using Graphics Processing Units*, Contributed Poster at TDDFT Summer School, Benasque, Spain, (September, 2008)

11. *Accelerating Quantum Chemistry Using Graphics Processing Units*, Invited Talk at National Institutes of Health, Bethesda, MD. (May, 2008)

Organization and Participation

1. *Graduate Consortium on Energy and Environment*. First generation member of the consortium, Harvard University, Cambridge MA, USA (January 2009).

2. *Harvard University Mexican Association*.

   - Internal Vice-president (June, 2010-June, 2011)
   - GSAS Representative (June, 2009-June, 2010)

Graduate Coursework

Energy Policy Analysis	*Spring 2010*
The Consequences of Energy Systems	*Fall 2009*
Survey of Energy Technology	*Spring 2009*
Advanced Electromagnetism	*Fall 2008*
Applied Quantum Mechanics	*Spring 2008*
Statistical Thermodynamics	*Fall 2007*
Advanced Quantum Mechanics I	*Fall 2007*
Quantum Computation	*Fall 2007*

Technical Skills

Programming Languages C, Fortran, Python, Matlab, R, Mathematica, Perl, MySQL, Visual Basic, PHP, HTML, and others.

Computational Chemistry Software Q-Chem (Developer), Octopus (Developer), Turbomole, CHARMM

Hardware Built and administer Jabba, a 90 TB storage array for the Clean Energy Project

Languages	Fluent in *Spanish*, *English* and *German*.
General Information	Born on April 3rd, 1983 at Mexico City, Mexico. Citizenship: *Mexican*
References	*Prof. Alan Aspuru-Guzik* Harvard University, Department of Chemistry and Chemical Biology 12 Oxford Street, Room M113, Cambridge, MA 02138 Email: alan@aspuru.com Tel: (617) 384-8188, Fax: (617) 496-9411 *Prof. Carlos Amador-Bedolla* Facultad de Qumica, Universidad Nacional Autónoma de México Posgrado, Edificio B, Ciudad Universitaria, Mxico D. F. 04510 México Email: carlos.amador@unam.mx Tel: +52-55-56223767 *Dr. Michael Stopa* Physics Department, Center for Nanoscale Systems 11 Oxford Street, Cambridge, MA 02138 Email: stopa@cns.fas.harvard.edu Tel: (617)-496-6932 *Dr. Mark A. Watson* Harvard University, Department of Chemistry and Chemical Biology 12 Oxford Street, Room M135, Cambridge, MA 02138 Email: mark@seas.harvard.edu Tel: (617)-496-8221