DR. MARISOL ALCÁNTARA ORTIGOZA
CURRICULUM VITAE

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RESEARCH EXPERIENCE

- **Department of Physics, University of Central Florida**, Orlando, FL, USA
  08/2012 – present — Research Associate

- **Donostia International Physics Center**, Donostia-San Sebastián, Spain
  07/2013 – 08/2012, 12/2014 – 12/2015 — Visiting Scientist

- **Institut für Festkörperphysik, Karlsruher Institut für Technologie**, Germany
  2005- 2008: summer stays — Visiting Scientist
  05/2009 – 10/2009
  10/2010 – 02/2011
  10/2011 – 11/2011

- **Department of Physics, University of Central Florida**, Orlando, FL, USA
  10/2007 – 08/2012 — Postdoctoral Research Associate

- **Department of Physics, Kansas State University**, Manhattan, KS, USA
  08/2002 – 08/2007 — Graduate Research Assistant

- **Centro de Ciencias Físicas, Universidad Nacional Autȯnoma de México**, Cuernavaca, México
  2000 – 2001 — Undergraduate Research Assistant

TEACHING EXPERIENCE

- **Department of Physics, University of Central Florida**, Orlando, FL, USA
  08/2013 – 05/2014
  Experience with both traditional lecture and new Mini-Studio modes.

- **Department of Physics, Kansas State University**, Manhattan, KS, USA
  2001 – 2002 — Graduate Teaching Assistant

- **Facultad de Ciencias, Universidad Nacional Autȯnoma de México**, Ciudad de México, México
  1999 – 2001 — Undergraduate Instructor

EDUCATION

- **Ph.D. in Physics** (Condensed Matter Physics), December 7, 2007

Kansas State University, Physics Department, Manhattan, Kansas, USA
Advisor: Prof. Talat S. Rahman
Thesis: "Theoretical studies of electronic, vibrational, and magnetic properties of chemisorbed surfaces and nanoalloys."

- **Bachelor in Physics** (Thesis in Atomic Physics), June 2001

Universidad Nacional Autónoma de México, Facultad de Ciencias, Mexico City, Mexico.
Advisor: Prof. Horacio Martínez Valencia
Thesis: "Sección transversal y umbral de energía de la producción de rayos X en colisiones ion-átomo."

SYNERGISTIC ACTIVITY

- Contributor to the NSF-supported project: "Active Learning Strategies for Algebra-based Introductory Physics at UCF" (Award Number: 1246024) by teaching in the Mini-Studio for non-science, -technology, -engineering, and –math (non-STEM) students and designing worksheets focused on concepts, critical thinking and physics' broad landscape.
- Chair for the Session on "Quantum Condensed Matter Systems" at the 35th International Nathiagali Summer College on Physics and Contemporary Needs, Nathiagali, Pakistan, June 28-July4, 2010.
- Referee of manuscripts for Physical Chemistry Chemical Physics (PCCP), Journal of Chemical Physics, Journal of Physics: Condensed Metter, and Computational Material Science.

MEMBERSHIPS

- 2005 – present – Member of the American Physics Society
- 2010 – present – Member of the American Vacuum Society
- 2009 – present – Member of the American Harp Society

PUBLICATIONS

1. **M. Alcántara Ortigoza**, R. Heid, T. S. Rahman, K.P. Bohnen; "A closer look at how symmetry constraints and the spin-orbit coupling shape the electronic structure of Bi(111)"; In preparation.

2. **M. Alcántara Ortigoza**, M. Aminpour and T. S. Rahman; "Friedel oscillations responsible for stacking fault of adatoms: The case of Mg(0001) and Be(0001)"; Submitted to Physical Review B, December (2014).

3. **M. Alcántara Ortigoza** and S. Stolbov; "Lattice perturbation: The missing key to understand gold "nobleness""; Submitted to Journal of Chemical Physics, October (2014).

4. S. Stolbov and **M. Alcántara Ortigoza**; "Gold-doped Graphene: a Highly Stable and Active Electro-catalysts for the Oxygen Reduction Reaction"; Revision submitted to Journal of Physical Chemistry C; August (2014).

5. **M. Alcántara Ortigoza**, I. Yu. Sklyadneva, R. Heid, E. V. Chulkov, T. S. Rahman, K.P. Bohnen, and P. M. Echenique; "Ab initio lattice dynamics and electron-phonon coupling of Bi(111)"; Phys. Rev. B **90**, 195438 (2014).

6. **M. Alcántara Ortigoza**, M. Aminpour and T. S. Rahman; "Revisiting the surface properties of Mg(0001) thin films and their effect on the adatom binding energy and self-diffusion"; *Surface Science*, **632**, 14-19 (2015).

7. **M. Alcántara Ortigoza**, R. Heid, K. P. Bohnen, and T. S. Rahman; "Anomalously Soft and Stiff Modes of Transition-Metal Nanoparticles"; *J. Phys. Chem. C,* **118** , 10335 (2014).

8. T. Tomanic, C. Sürgers, R. Heid, **M. Alcántara Ortigoza**, K.-P. Bohnen, D. Stöffler, and H. v. Löhneysen; "Local-strain mapping on Ag(111) islands on Nb(110)", Appl. Phys. Lett. **101**, 063111 (2012).

9. D. Sun, W. Lu, D. Le, Q. Ma, M. Aminpour, **M. Alcántara Ortigoza**, S. Bobek, J. Mann, J. Wyrick, T. S. Rahman, and L. Bartels; "An MoS_x Structure with High Affinity for Adsorbate Interaction", Angew. Chem. Int. Ed. 51, 10284 (2012).

10. S. Stolbov and **M. Alcántara Ortigoza**; "Rational Design of Competitive Electrocatalysts for Hydrogen Fuel Cells", *J. Phys. Chem. Letts.* **3**, 463 (2012).

11. G. S. Shafai, **M. Alcántara Ortigoza**, and T. S. Rahman; "Is the Debye-temperature a useful concept at the nanometer scale? Insights from ab initio free energy calculations of Au_{13} and $Au_{12}Fe$ nanoclusters", J. Phys.: Condens. Matter **24**, 104026 (2012).

12. B. Roldán Cuenya, **M. Alcántara Ortigoza**, L. K. Ono, F. Behafarid, S. Mostafa, J. R. Croy, K. Paredis, G. Shafai, T. S. Rahman, L. Li, Z. Zhang, and J. C. Yang, "Thermodynamic properties of Pt nanoparticles: Size, shape, support, and adsorbate effects"; Phys. Rev. B **84**, 245438 (2011).

13. **M. Alcántara Ortigoza**, R. Heid, K. P. Bohnen, and T. S. Rahman, "Nature of the Binding of a c(2x2)-CO Overlayer on Ag(001) and Surface Mediated Intermolecular Coupling"; *J. Phys. Chem. A,* **115** (25), 7291 (2011).

14. **M. Alcántara Ortigoza**, T. S. Rahman, R. Heid, and K. P. Bohnen, "Ab initio Calculations of the Dispersion of Surface Phonons of a c(2x2) CO overlayer on Ag(001)"; *J. Phys.: Condens. Matter* **22**, 395001 (2010).

15. S. S. Hayat, **M. Alcántara Ortigoza**, M. A. Choudhry, and T. S. Rahman, "Diffusion of Cu monomers and dimers on Ag(111): Molecular dynamics simulations and density functional theory calculations"; *Phys. Rev.* B **82**, 085405 (2010).

16. E. Z. Ciftlikli, L. V. Goncharova, B. J. Hinch, **M. Alcántara Ortigoza**, S. Hong, T. S. Rahman, "Vibrational dynamics of a c(2×2) phase induced by nitrogen adsorption

on Cu(001)"; Phys. Rev. B **81**, 115465 (2010).

17. **M. Alcántara Ortigoza**, R. Heid, K. P. Bohnen, and T. S Rahman, "Effect of c(2x2)-CO overlayer on the phonons of Cu(001): A first-principles study"; *Phys. Rev.* B **79**, 125432 (2009).

18. S. Stolbov, **M. Alcántara Ortigoza**, R. R. Adzic, and T. S. Rahman, "High CO tolerance of Pt/Ru nano-catalyst: Insight from first principles"; *J. Chem. Phys*. **130**, 124714 (2009).

19. S. Stolbov, **M. Alcántara Ortigoza**, and T. S. Rahman; "Application of density functional theory to CO tolerance in fuel cells: a brief review"; *J. Phys.: Condens. Matter* **21**, 474226 (2009).

20. **M. Alcántara Ortigoza**, S. Stolbov, and T. S. Rahman, "Formation of Pt islets on facets of Ru nanoparticles: First-principles study"; *Phys. Rev.* B **78**, 195417 (2008).

21. **M. Alcántara Ortigoza** and T. S. Rahman; "First principles calculations of the electronic and geometric structure of $Ag_{27}Cu_7$ nanoalloy", *Phys. Rev.* B **77**, 195404 (2008).

22. **M. Alcántara Ortigoza** and T. S. Rahman; "Symmetry and novelty in the electronic and geometric structure of nanoalloys: the case of $Ag_{27}Cu_7$"; Contemporary Physics: Proceedings of the International Symposium by Jamil Aslam, Faheem Hussain, Riazuddin; Published by World Scientific (2008).

23. **M. Alcántara Ortigoza**, T. S. Rahman, R. Heid, and K. P. Bohnen; "First-principles study of the lattice dynamics of c(2 × 2)-CO on Cu(001)", *J. Phys.: Condens. Matter* **20**, 224009 (2008).

24. **M. Alcántara Ortigoza**, R. A. Klemm, T. S. Rahman, Comment on "Magnetization of two-dimensional square arrays of nanomagnets", *Phys. Rev.* B **74**, 226401 (2006).

25. **M. Alcántara Ortigoza**, R. A. Klemm, T. S. Rahman, "Effect of dipolar interactions on the magnetization of a cubic array of nanomagnets", *Phys. Rev.* B **72**, 174416 (2005).

INVITED TALKS

1. Novel pathways in the rational design of materials: an application to clean energy conversion; XXIII International Materials Research Congress, Cancun, Quintana Roo, August 2014.

2. How “nano” is nanoscience?; NanoMex 2012, Puebla, Mexico, June 14th, 2012.

3. Vibrational dynamics and diffusion of CO on metal surfaces: New answers to old questions using *ab initio* atomistic simulations; European Conference on Surface Science XXVII, Groningen, Netherlands, September 1st, 2010.

4. *Ab initio* vibrational dynamics applied to analyze the CO-metal (Cu,Ag) coupling; 13th Vibrations at Surfaces meeting, Orlando, Florida, USA, March 13, 2010.

5. Formation of bilayer islands in heteroepitaxy of transition metals: insights from first principles calculations; Session on Scientific Computing and Mathematical Modeling within the 35th International Nathiagali Summer College on Physics and Contemporary Needs, Nathiagali, Pakistan, July 4-July 10, 2010.

6. Formation of Pt islands on Ru nanoclusters Insights from *ab initio* calculations; Session on Scientific Computing and Mathematical Modeling within the 35th International Nathiagali Summer College on Physics and Contemporary Needs, Nathiagali, Pakistan, July4-July 10, 2010.

7. Modeling and Design of Materials from the Perspective of the Density Functional Theory: Basics and Selected Applications; Session on Quantum Condensed Matter Systems within the 35th International Nathiagali Summer College on Physics and Contemporary Needs, Nathiagali, Pakistan, June 28-July4, 2010.

CONTRIBUTED PRESENTATIONS

1. Novel pathway for the rational design of materials: An application to clean energy conversion: Special Seminar, Instituto de Física, Universidad Nacional Autónoma de México, April 1st, 2014.
2. Mg(0001): Electronic structure features controlling the limit of and reactivity in the thin-film regime, stacking fault of Mg adislands and adatom self-diffusion: American Physical Society Meeting, Denver, Colorado, USA, March 5th, 2014.
3. Origin and application of the ``lattice distortion energy'' spent upon chemisorption: Poster at American Physical Society Meeting, Denver, Colorado, USA, March 5th, 2014.
4. Vibrational spectrum and stability of the long-debated models for the $(7\sqrt{}\times7\sqrt{})R19^{\circ}$ phase of S/Cu(111): Poster at American Physical Society Meeting, Denver, Colorado, USA, March 4th, 2014.
5. The unsuspected origin of gold's nobleness: Condensed Matter Physics Seminar, Physics Department, University of Central Florida, April 22th, 2013.
6. Stabilizing and enhancing activity of Ag as a catalyst for oxygen redaction reaction on hydrogen fuel cell cathodes: American Physical Society Meeting, Baltimore, Maryland, USA, March 18, 2013.
7. The unsuspected origin of gold's nobleness: American Physical Society Meeting, Baltimore, Maryland, USA, March 19, 2013.
8. Factors controlling the thermodynamic properties at the nanoscale: Ab initio study of Pt nanoparticles: American Vacuum Society Symposium, Tampa, Florida, USA, October 28 - November 2, 2012.
9. Rational Design of Competitive Electrocatalysts for Hydrogen Fuel Cells: American Vacuum Society Symposium, Tampa, Florida, USA, October 28 - November 2, 2012.
10. First-principles investigation of the stability and vibrational spectrum of MoSx nanostructures grown on Cu(111): American Vacuum Society Symposium, Tampa, Florida, USA, October 28 - November 2, 2012.
11. Vibrational spectrum and stability of the long-debated models for the $(\sqrt{7}\times\sqrt{7})R19^{\circ}$

phase of S/Cu(111): American Vacuum Society Symposium, Tampa, Florida, USA, October 28 - November 2, 2012.

12. Factors controlling thermodynamic properties at the nanoscale: Ab initio study of Pt nanoparticles: American Physical Society Meeting, Boston, Massachusetts, USA, March 1st, 2012.
13. Insights on the electronic and vibrational properties of Bi(111) from first principles: American Physical Society Meeting, Boston, Massachusetts, USA, February 28th, 2012.
14. Insights on the "topological insulator phase" and anomalous lattice dynamics of Bi(111): Condensed Matter Physics Seminar, Physics Department, University of Central Florida, March 7th, 2012.
15. Electronic structure and lattice dynamics of Bi(111): Insights from ab initio calculations: Colloquium of the Institut für Festkörperphysik, Karlsruher Institut für Technologie (Campus Süd), Karlsruhe, Germany, November 28, 2011.
16. Electronic Structure of Bi(111): Clarification of the role of the spin-orbit coupling, Florida Society of Material Simulation Annual Meeting, University of Central Florida, August 1-2 ,2011.
17. Interpreting the unexpected outcome of measurements at the nanoscale: ab initio thermodynamic properties, Condensed Matter Physics Seminar, Physics Department, University of Central Florida, April 11st, 2011.
18. Insights on the anomalously soft and stiff modes of metal nanoparticles; American Physical Society Meeting, Dallas, Texas, USA, March 24th, 2011.
19. Is the Debye-temperature a useful concept at the nanometer scale? Insights from *ab initio* free energy calculations of Au_{13} and $Au_{12}Fe$ nanoclusters; American Physical Society Meeting, Dallas, Texas, USA, March 24th, 2011.
20. Bilayer islands in heteroepitaxy of transition metals: insights from first principles; American Physical Society Meeting, Dallas, Texas, USA, March 23th, 2011.
21. *Ab initio* study of Mg self-diffusion on Mg(0001) terraces and steps; American Physical Society Meeting, Dallas, Texas, USA, March 22th, 2011.
22. Nature of Binding and Vibrational Dynamics of CO on metal surfaces: answers to old questions using *ab initio* calculations; Poster at Gordon Research Conferences on Chemical Reactions at Surfaces; Ventura California, February 6-11, 2011.
23. On the transition from bulk to nanoparticles: First-principles vibrational dynamics; Seminar of the Institut für Festkörperphysik, Karlsruher Institut für Technologie (Campus Nord), Eggenstein, Germany, November 4th, 2010.
24. *Ab initio* calculations of pre-exponential factors for the diffusion of CO on Ag(001): importance of the full phonon dispersion; American Vacuum Society 57th Meeting, Albuquerque, New Mexico, USA, October 19th , 2010.
25. Vibrational dynamics and diffusion of CO on metal surfaces: New answers to old questions using *ab initio* atomistic simulations; Colloquium of the Department of Physics, Karlsruher Institut für Technologie (Campus Süd), Karlsruhe, Germany, October 18th, 2010.
26. *Ab initio* calculations of the "pre-exponential factor" for the diffusion of CO on Ag(001): importance of the full phonon dispersion; American Physical Society Meeting, Portland, Oregon, USA, March 16 2010.
27. *Ab initio* study of size effects on Mg thin films and Mg self-diffusion on wide vs. narrow (0001) terraces; Poster at NanoFlorida 2010, Orlando, Florida, USA, September 10, 2010.
28. Is the Debye-temperature a useful concept at the nanometer scale?: insights from *ab initio* free energy calculations of Au_{13} and $Au_{12}Fe$ nanoclusters, Poster at

NanoFlorida 2010, Orlando, Florida, USA, September 10, 2010.

29. Formation of bilayer islands in heteroepitaxy on transition metals: insights from first principles calculations, NanoFlorida 2010, Orlando, Florida, USA, September 10, 2010.
30. Formation of bilayer islands in heteroepitaxy of transition metals: insights from first principles calculations; Condensed Matter Physics Seminar, Physics Department, University of Central Florida, April 21st, 2010.
31. *Ab initio* calculations of the "pre-exponential factor" for the diffusion of CO on Ag(001): importance of the full phonon dispersion; American Physical Society Meeting, Portland, Oregon, USA, March 16, 2010.
32. Vibrational Dynamics of c(2x2) CO overlayer on Cu(100) and Ag(100) from first principles; Seminar at the Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany, July 30, 2009.
33. First-principles study of the lattice dynamics of c(2 × 2)-CO on Cu(001); Florida Chapter of the AVS Science and Technology Society, Orlando, Florida, USA, March 8 2009.
34. *Ab initio* vibrational dynamics of Ag27Cu7 nanoalloy; American Physical Society Meeting, Pittsburgh, Pennsylvania, USA, March 17 2009.
35. Diffusion of two-dimensional Cu islets on Ag(111) studied with the Molecular Dynamics Method; American Physical Society Meeting, Pittsburgh, Pennsylvania, USA, March 17 2009.
36. Vibrational spectroscopy and ab initio dynamics of the O-induced added-row reconstructed Cu(110) surface; American Physical Society, March Meeting, New Orleans, Louisiana, 2008.
37. First principles calculations of the vibrational dynamics of c(2x2)-CO on Ag(001); American Physical Society, March Meeting, New Orleans, Louisiana, 2008.
38. Insights into the stability of $Ag_{27}Cu_7$ nanoalloy from first principles calculations of geometric and electronic structure, A mid-time Conference of the COST Action p19: Multiscale Modelling of Materials, Brno, Czech Republic, June 2008.
39. First-Principles Study of the Lattice Dynamics of c(2x2)-CO on Cu(001); Seminar at the Insitut für Festkörperphysik of the Forschungszentrum Karlsruhe, Germany, July 24 2008.
40. First principles vibrational dynamics of c(2x2)-CO on Ag(001); First Annual Nanoscience Technology Symposium, NANOFLORIDA, University of Central Florida, Orlando, Florida, USA, September 2008.
41. Insights into the stability of $Ag_{27}Cu_7$ nanoalloy from first principles calculations of geometric and electronic structure; First Annual Nanoscience Technology Symposium: NANOFLORIDA, University of Central Florida, Orlando, Florida, USA, September 2008.
42. The importance of the dipolar interaction strength in magnetization hysteresis curves of two-dimensional nanomagnet arrays; Denver CO, American Physical Society, March Meeting, 2007.
43. First principles studies of the geometric and electronic structure of nanoalloy $Ag_{27}Cu_7$; Denver CO, American Physical Society, March Meeting, 2007.
44. Formation of Pt nano-islands on Ru(0001) surface: insights from *ab initio* calculations, Denver CO; American Physical Society, March Meeting, 2007.
45. Formation of Pt islands on Ru nanoclusters; Condensed Matter Physics Seminar, Physics Department, University of Central Florida, March 26th, 2007.
46. Diffusion of Dimers in Complex Geometries: Density Functional Theory Calculations; The 3rd Annual Workshop on Self-Learning Kinetic Monte Carlo,

Department of Physics, University of Central Florida, April 28, 2007.

47. The dispersion of surface phonons of CO on Cu(100): insights from first-principles calculations; Vibrations at surfaces 12, XII International Conference, Erice, Italy, July 24th 2007.
48. Effect of the substrate-adsorbate coupling on the dispersion of phonons of CO on Cu(001); American Physical Society, March Meeting, Baltimore MD, 2006.
49. Effect of dipolar interactions on the magnetization of a cubic array of nanomagnets, Baltimore MD, American Physical Society, March Meeting, 2006.
50. First principles studies of the geometric and electronic structure of nanoalloy $Ag_{27}Cu_7$; Summer School on Metal Clusters and Surfaces, Pisa, Italy, 2006.
51. Bimetallic system: application on fuel cells; Condensed Matter Physics Seminar, Physics Department, Kansas State University, 2006.
52. First Principles Studies of the Reactivity of Pt Islets on Ru(0001); AVS 53rd International Symposium, San Francisco CA, 2006.
53. Effect of Dipolar Interactions on the Magnetization of Single-Molecule Magnets in a cubic lattice; American Physical Society, March Meeting, Los Angeles CA, 2005.
54. Hysteresis by cubic arrays of nanomagnets under dipolar interactions; Condensed Matter Physics Seminar, Physics Department, Kansas State University, 2005.
55. Effect of Dipolar Interaction in Magnetization of Classical SMM in a cubic lattice; Condensed Matter Physics Seminar, Physics Department, Kansas State University, 2004.
56. Dipolar interaction between Single Molecule Magnets (SMM) in a 2D hexagonal lattice; Condensed Matter Physics Seminar, Physics Department, Kansas State University, 2003.
57. Cálculo y comparación experimental de la sección transversal de la pérdida electrónica de átomos Rydberg usando la aproximación de Born; Poster at the XLIII Congreso Nacional de Física, Puebla, México, 2000.

COLLABORATORS:

- Prof. Talat S. Rahman, Department of Physics, University of Central Florida, Orlando, Florida 32816, USA
- Prof. Sergey Stolbov, Department of Physics, University of Central Florida, Orlando, Florida 32816, USA
- Dr. Klaus Peter Bohnen, Institut für Festkörperphysik, Karlsruher Institut für Technologie, Eggenstein-Leopoldshafen 76344, Germany
- Dr. Rolf Heid, Institut für Festkorperphysik, Karlsruher Institut für Technologie, Eggenstein-Leopoldshafen 76344, Germany
- Dr. Christian Ast, Max-Planck-Institute for Solid State Research, Heisenbergstr. 1, D-70569, Stuttgart , Germany
- Prof. Beatriz Roldán Cuenya, Department of Physics, University of Central Florida, Orlando, Florida 32816, USA
- Prof. Richard A. Klemm, Department of Physics, University of Central Florida, Orlando, Florida 32816, USA
- Prof. Jane Hinch, Department of Chemistry and Chemical Biology, Rutgers University, Piscataway, New Jersey 08854, USA
- Dr. Sadar S. Hayat, Department of Physics and Astronomy, Hazara

University Mansehran (NWFP), Pakistan.
- Prof. Maki Kawai, Surface Chemistry Laboratory, RIKEN, 2-1 Hirosawa, Wako, Saitama 351-0198, Japan.
- Prof. Yousoo Kim, Surface Chemistry Laboratory, RIKEN, 2-1 Hirosawa, Wako, Saitama 351-0198, Japan.