

# Curriculum Vitae

– August 2014 –

## Xóchitl López-Lozano

Assistant Professor

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## EDUCATIONAL BACKGROUND

[Jul.21, 2005] **Ph.D. in Sciences (Physics)**

Institute of Physics “*Ing. Luis Rivera Terrazas*”, Meritorious Autonomous University of Puebla (IF-BUAP), Puebla, Pue., Mexico, on **Scholarship** by the National Council of Science and Technology of Mexico (CONACyT).

Thesis (in Spanish): *Electronic and Optical Properties of InAs(110) Surface and Atomic Wires of In/Si(111)*.

Advisors: Dr. Cecilia Noguez Garrido, Institute of Physics, National Autonomous University of Mexico (IF-UNAM) and Dr. Lilia Meza Montes, IF-BUAP.

[Oct.2003-May.2004] **Research visit** in the group of Prof. Friedhelm Bechstedt at the Institute of Condensed Matter Theory and Solid State Physics of the Friedrich-Schiller University of Jena, Jena, Germany. Topic: *Ab Initio Study of In Nanowires on Si(111) Surface*.

[Dec.14, 2001] **Master degree (M.Sc.)** (Non-thesis option, i.e., General Exams)

IF-BUAP, Puebla, Pue., Mexico, on **Scholarship** by CONACyT.

[Jun.15, 2001] **Bachelor degree (B.Sc.)**

Facultad de Ciencias Físico-Matemáticas, Meritorious Autonomous University of Puebla (FCFM-BUAP), Puebla, Pue., Mexico.

Topic: Classical Dynamics of Non-Linear Systems and Chaos.

Thesis (in Spanish): *Classical Dynamics of a Particle in a Combined Parabolic and Coulombian Potential*.

Advisor: Dr. Germán A. Luna Acosta, IF-BUAP.

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## PROFESSIONAL EMPLOYMENT HISTORY

[Aug.18, 2009 - Present] **Tenure-Track Assistant Professor**. Department of Physics and Astronomy, The University of Texas at San Antonio, San Antonio, TX, USA.

[Nov.15, 2006 - Jul.31, 2009] **Postdoctoral Research Position**. Theoretical spectroscopy group of Dr. Lucia Reining, Paris node of the European Theoretical Spectroscopy Facility (ETSF) at the Laboratoire des Solides Irradiés of the École Polytechnique, Palaiseau, France.

Topic1: *Wave-Vector-Dependence Study of the Optical Response of Small Carbon Nanotubes*.

Topic2: *Ab Initio Study of the Structural and Electronic Properties of MoS<sub>2</sub> Nanoplatelets*.

[Aug.01, 2005 - Nov.01, 2006] **Postdoctoral Research Position**. Department of Complex Systems in the group of Dr. Ignacio Luis Garzón Sosa, IF-UNAM, Mexico.

Topic: *Ab Initio Studies of the Structural and Electronic Properties of Chiral Au Nanoclusters*.

## RESEARCH AREA AND INTERESTS

Condensed Matter Theory; Physics of Nanostructures; Optical spectroscopy;  
Total energy calculations and structure optimization using Density Functional Theory.

Theoretical study and atomic scale materials modeling, e.g., electronic structure calculations from first principles, of low-dimensional nanostructures with high potential for scientific and technological applications in the areas of Catalysis, Plasmonics and Chemistry, among others. Specifically, investigate and design the properties of materials at the nanometer scale using semi-empirical and *ab initio* density-functional theory calculations (DFT), and the experimental results, mainly from current collaborators. The main focus has been on the fundamental understanding and the tuning of the optical response of nanoparticles (bare, thiol-protected, nanoalloys, etc.) using time-dependent DFT (TDDFT). I also investigate the properties of MoS<sub>2</sub> nanostructures to understand and establish the relationship between the structural properties and the catalytic activity.

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## AWARDS AND HONORS

**Tenure-Track Research Award Competition FY 2012-2013** granted by The University of Texas at San Antonio, TX, USA. \$22,000 grant to stimulate junior faculty to perform research in their area of interest.

Member of the **SNI** (National System of Researchers) in Mexico since January 1<sup>st</sup>, 2007: **Level I**

**Postdoctoral Fellowship Award 2008-2009** granted by CONACyT on the category of *Consolidation of Research Groups*, within the framework of the convocation to support the Enhancement of the National Graduate Quality, the Consolidation of Research Groups and Technological Capacity of Enterprises.

**Hosting Institution:** Theoretical spectroscopy group of Dr. Lucia Reining, Paris node of the European Theoretical Spectroscopy Facility (ETSF) at the Laboratoire des Solides Irradiés of the École Polytechnique, Palaiseau, France.

**Project Title:** *Optical Properties of Carbon Nanotubes: Study of the Momentum-Transfer Dependence.*

Award **IIM-UNAM 2006** granted by the National Autonomous University of Mexico for **the best PhD thesis in the field of science and engineering in Mexico.**

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## RESEARCH & SCHOLARLY ACTIVITIES SUMMARY

**Number of Peer-Reviewed Publications 2009 – 2014: 12**

**Proceedings: 1**

**Articles in Preparation: 3**

**Total Number of Peer-Reviewed Publications since 1998: 18 ; Total Proceedings: 5**

### List of Publications

– 2014 –

- [1] *Optical Response of Quantum-Sized Ag and Au Clusters – Cage vs. Compact Structures and the Remarkable Insensitivity to Compression.*

H.-Ch. Weissker, R. L. Whetten and **X. López-Lozano**

Phys. Chem. Chem. Phys. 16, 12495-12502, **2014**. DOI: 10.1039/C4CP01277A

**Corresponding Author: X. López-Lozano**

- [2] *Information on Quantum States Pervades the Visible Spectrum of the Ubiquitous Au<sub>144</sub>(SR)<sub>60</sub> Gold Nanocluster.*  
H.-Ch. Weissker, H. Barrón, V. D. Thanthirige, K. Kwak, D. Lee, G. Ramakrishna, R. L. Whetten and **X. López-Lozano**, Nature Communications 5, 3785, 1-8, **2014**. DOI:10.1038/ncomms4785  
**Corresponding Authors: H.-Ch. Weissker and X. López-Lozano.**
- [3] *Systematic Study of the Adsorption of Thiol Molecules on a Au<sub>55</sub> Nanoparticle.*  
H. Barrón, L. Fernández-Seivane and **X. López-Lozano**.  
Phys. Stat. Sol. (B), No. 6, 1239-1247, **2014**. DOI: 10.1002/pssb.201350183  
**Corresponding Author: X. López-Lozano**
- [4] *Aspect-Ratio- and Size-Dependent Emergence of the Surface-Plasmon Resonance in Gold Nanorods – an Ab Initio TDDFT Study.*  
**X. López-Lozano**, H. Barrón, C. Mottet, and H.-Ch. Weissker.  
Phys. Chem. Chem. Phys. (Communication) 16, 1820-1823, **2014**. DOI: 10.1039/c3cp53702a  
**Corresponding Author: X. López-Lozano**

– 2013 –

- [5] *Trends and Properties of 13-Atom Ag–Au Nanoalloys I: Structure and Electronic Properties*  
H. Barrón, L. Fernández-Seivane, H.-Ch. Weissker and **X. López-Lozano**.  
J. Phys. Chem. C 117, 21450-21459, **2013**. DOI: 10.1021/jp403230t  
**Corresponding Author: X. López-Lozano**
- [6] *Effect of Alloying on the Optical Properties of Ag–Au Nanoparticles.*  
**X. López-Lozano**, C. Mottet, and H.-Ch. Weissker.  
J. Phys. Chem. C 117, 3062-3068, **2013**. DOI: 10.1021/jp309957y  
**Corresponding Author: X. López-Lozano**
- [7] *Atomic and Electronic Properties of Quasi-One Dimensional MoS<sub>2</sub> Nanowires.*  
L. Fernández-Seivane, H. Barrón, S. Botti, M. Marques, A. Rubio and **X. López-Lozano**.  
**Invited Feature Paper.** Journal of Materials Research. Vol. 28, No. 2, 240-249, **2013**.  
DOI: 10.1557/jmr.2012.355  
**Corresponding Author: X. López-Lozano**

– 2012 –

- [8] *Insights Into the Structure of MoS<sub>2</sub>/WS<sub>2</sub> Nanomaterial Catalysts as Revealed by Aberration Corrected STEM.*  
F. L. Deepak, R. Esparza, C. F. Castro-Guerrero, S. Mejía, **X. López-Lozano**, M. José-Yacamán.  
Microscopy and Microanalysis, Vol. 18 (Suppl. 5), **2012**. DOI:10.1017/S1431927612012986

– 2011 –

- [9] *Rippled and Helical MoS<sub>2</sub> Nanowire Catalysts - An Aberration Corrected STEM Study.*  
F. L. D., R. Esparza, B. Borges, **X. López-Lozano** and M. José-Yacamán. Catal. Lett. **141**, 518-524, **2011**. DOI: 10.1007/s10562-011-0550-1.
- [10] *Direct Imaging and Identification of Individual Dopant Atoms in MoS<sub>2</sub> and WS<sub>2</sub> Catalysts by Aberration Corrected STEM study.*  
F. L. Deepak, R. Esparza, B. Borges, **X. López-Lozano**, M. José-Yacamán. ACS Catal., 1 (5), 537543, **2011**. DOI:10.1021/cs100141p
- [11] *Experimental and Theoretical Properties of S–Mo–Co–S Clusters.*  
D.H. Galvan, F. L. Deepak, R. Esparza, A. Posada-Amarillas, R. Núñez-González, **X. López-Lozano** and M. José-Yacamán. Applied Catalysis A: General **397** (1), 46-53, **2011**.  
DOI: 10.1016/j.apcata.2011.02.010

– 2009 –

- [12] *Density Functional Study of the Cysteine Adsorption on Au Nanoclusters.*  
L. A. Pérez, **X. López-Lozano** and I. L. Garzon, Eur. Phys. J. D **52**, 123-126, **2009**.

#### Proceedings.

- [13] *Optical Properties of Bimetallic Nanoalloys from TDDFT – Absorption Spectra of 13-Atom Noble Metal Clusters.*  
H.-Ch. Weissker, H. Barrón, L. Fernández-Seivane and **X. López-Lozano**.  
Proceedings of International Conference Nanomeeting – 2013, Physics, Chemistry and Applications of Nanostructures, Minsk, Belarus, 28 – 31 May 2013. Published by World Scientific Publishing Co. Pte. Ltd., **2013**. ISBN #9789814460187, pp. 121-123. DOI:10.11429789814460187\_0029

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#### ARTICLES IN PREPARATION: 3

- [14] *Optical Properties of Small Ag–Au Nanoalloys.*  
A. Canales, A. Salgado, H. Barrón, S. Clark, L. Fernández-Seivane and **X. López-Lozano**.
- [15] *Perspectives on the Physical Chemistry of the Ubiquitous Icosahedral Clusters Comprising 145 Noble-Metal Sites and 60 Ligands.*  
Robert L. Whetten, A. Tlahuice-Flores, N. Bhattarai, **X. López-Lozano**, H.-Ch. Weissker, D. M. Black, S. B. Bach, M. Jose-Yacamán.
- [16] *Trends and Properties of 13-Atom Ag–Au Nanoalloys II: Optical Properties.*  
H. Barrón, L. Fernández-Seivane, H.-Ch. Weissker and **X. López-Lozano**.

July 2014. Invited to submit an article to The Journal of Physical Chemistry's Special Issue entitled: **Current Trends in Clusters and Nanoparticles.**

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#### Publications – 2003 - 2006 –

- [17] *Enantiospecific Adsorption of Chiral Molecules on Chiral Au Clusters.*  
**X. López-Lozano**, L. A. Pérez and I. L. Garzon. Phys. Rev. Lett. **97**, 223401, 2006.  
Included in the Virtual Journal of Nanoscale Science and Technology.
- [18] *Reconstruction of Quasi-1D In/Si(111) System: Charge and Spin Density Waves versus Bonding.*  
**X. López-Lozano**, A. Krivosheeva, A. A. Stekolnikov, L. Meza-Montes, C. Noguez, J. Furthmüller and F. Bechstedt, Phys. Rev. B **73**, 035430, 2006.  
Included in the Virtual Journal of Nanoscale Science and Technology.
- [19] *Band Structure and Electron Gas of In Chains on Si(111).*  
**X. López-Lozano**, A. A. Stekolnikov, J. Furthmüller and F. Bechstedt, Surf. Sci., **589**, 77-79, 2005.
- [20] *Electronic Structure and Reflectance Anisotropy Spectrum of InAs(110).*  
**X. López-Lozano**, O. Pulci, C. Noguez, K. Fleischer, R. del Sole and W. Richter, Phys. Rev. B **71**, 125337, 2005.
- [21] *Electronic and Optical Properties of InAs(110).*  
**X. López-Lozano**, C. Noguez and L. Meza-Montes, Rev. Mex. Fis., Vol. **51**, 168-175, 2005.

- [22] *Optical Properties of the Cleavage InAs(110) Surface*.  
**X. López-Lozano**, C. Noguez and L. Meza-Montes, Phys. Stat. Sol.(c) **0**, No. 8, 2992-2996, 2003.

**Proceedings – 2002 - 2007 –**

- [23] *Density Functional Study of the Cysteine Adsorption on Au Nanoparticles*.  
**X. López-Lozano**, L. A. Pérez and I. L. Garzon. 2007 NSTI Nanotechnology Conference and Trade Show - NSTI Nanotech 2007, Technical proceedings **4**, pp. 381-384, 2007.
- [24] *Quasi-1D In/Si(111) Surface Structures*.  
Andrey A. Stekolnikov, **Xóchitl López-Lozano**, Jürgen Furthmüller and Friedhelm Bechstedt, NIC Series, Vol. **32**, ISBN 3-00-017351-X, pp. 143-150, 2006. John von Neuman Institute for Computing, Jülich.
- [25] *Propiedades Electrónicas de Superficies Semiconductoras Ideales*.  
**X. López-Lozano**, C. Noguez and L. Meza-Montes, Textos Científicos BUAP. Memorias del V Taller Nacional de Física y Ciencia de Materiales para Estudiantes de Posgrado, BUAP, 99-103, 2003, ISBN: 968 863 683 5, Mexico.
- [26] *Propiedades Electrónicas de las Superficies Semiconductoras Ideales GaAs e InAs*.  
**X. López Lozano**, C. Noguez and L. Meza-Montes. Memorias del VIII Encuentro Regional de Investigación y Enseñanza de Física, 2002. (in CD)

**Other Publications.**

- [27] *La Conferencia Internacional sobre Mujeres en Física Organizada por la IUPAP*.  
L. Meza-Montes, **X. López Lozano** and A.M. Cetto. Boletín de la Sociedad Mexicana de Física, 2002. <http://www.ifuap.buap.mx/lilia/bolsmf.html>
- [28] *Mejorando la Participación de la Mujer en la Física: Un Esfuerzo Colectivo*.  
**X. López Lozano**, B. González and L. Meza-Montes. Memorias del VIII Encuentro Regional de Investigación y Enseñanza de Física, 2002. (in CD)

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## SCHOLARLY PRESENTATIONS

### A. CONFERENCE PRESENTATIONS

Conference Presentations 2009 – 2014: **39**

Orals: **16** ; Posters: **16** ; Invited Conference Talks: **7** ; Other Invited Talks: **5**

Total Presentations since 1998: **76**

Orals: **22** ; Posters: **38**; Total Invited Talks: **16**

\* – Presenter

– 2014 –

Sep.7-12, 2014 XVII ISSPIC, International Symposium on Small Particles and Inorganic Clusters. Fukuoka, Japan.  
**Hot Topic Talk:** *Surface Plasmons in Quantum-Sized Noble-Metal Clusters: Quantum Calculations and The Classical Picture of Charge Oscillations.*  
H.-Ch. Weissker\*, and X. López-Lozano.

**Poster:** *Information on Quantum States Pervades the Absorption Spectra of  $Au_{144}(SR)_{60}$  Nanocluster.* H.-Ch. Weissker, V. D. Thanthirige, K. Kwak, D. Lee, G. Ramakrishna, R. L. Whetten and X. López-Lozano\*.

Aug.17-21, 2014 XXIII IMRC (International Material Research Congress), Symposium 1A: Science of Atomic Clusters, Nanoparticles and their Assemblies. Materials Research Society, Cancun, Mexico.  
**Talk:** *Information on Quantum States Pervades the Absorption Spectra of  $Au_{144}(SR)_{60}$  Nanocluster.* H.-Ch. Weissker, V. D. Thanthirige, K. Kwak, D. Lee, G. Ramakrishna, R. L. Whetten and X. López-Lozano\*.

Jun.10-13, 2014 Meeting of the GDR Nanoalliges, Strasbourg, France.  
**Talk:** *Surface Plasmons in Real Time and the Classical Picture of Charge Oscillations: TDDFT Calculations.* H.-Ch. Weissker\* and X. López-Lozano.

Jun.2-4, 2014 Cluster Surface Interaction (CSI) Workshop 2014, Villa Cagnola, Gazzada Schianno (VA), Italy.

**Poster:** *Information on Quantum States Pervades in the Absorption Spectra of  $Au_{144}(SR)_{60}$  Nanocluster.* H.-Ch. Weissker, H. Barrón, V. D. Thanthirige, K. Kwak, D. Lee, G. Ramakrishna, R. L. Whetten and X. López-Lozano\*.

**Poster:** *Surface Plasmon in Real Time from Quantum Calculations and the Classical Picture of Charge Oscillations.* H.-Ch. Weissker\* and X. López-Lozano.

Apr.6-9, 2014 COST Action Meeting MP0903 NANOALLOY. Nanoalloys as Advanced Materials: From Structure to Properties and Applications. Workshop – Working groups 2 and 4. Santa Margherita Ligure, Italy.  
**Talk:** *Surface Plasmons in Real Time and the Classical Picture of Charge Oscillations from an Ab Initio TDDFT Calculations.* H.-Ch. Weissker\*, Christine Mottet, and X. López-Lozano.

– 2013 –

Oct.18, 2013 2013 COS (College of Sciences) Research Conference. Physics & Astronomy Session. The University of Texas at San Antonio, San Antonio, TX, USA.  
**Poster:** *Trends and Properties of 13-Atom Ag–Au Nanoalloys.* H. Barrón\*, L. Fernández-Seivane, H.-Ch. Weissker and X. López-Lozano.

Oct.1-4, 2013 18th ETSF Workshop on Electronic Excitations, Luxembourg, Luxembourg.  
**Poster:** *Surface Plasmons and Optical Response in Ag–Au Nanoalloys.* H.-Ch. Weissker\*, C. Mottet, H. Barrón, L. Fernández-Seivane, and X. López-Lozano.

Sep.15-20, 2013 7th International Conference on Theory of Atomic & Molecular Clusters (TAMC VII) Birmingham, England.  
**Talk:** *Surface Plasmon and Optical Response in Ag–Au Nanoalloys from Ab Initio TDDFT Calculations.* H.-Ch. Weissker\*, H. Barrón, L. Fernández-Seivane, and X. López-Lozano.

Jul.31-Aug.3, 2013 ISMPC13 – International Symposium on Monolayer Protected Cluster 2013, Pinyon Park Mountain Campus, Colorado State University, Colorado, USA.  
**Poster:** *Optical Properties of the Thiolate-Protected  $Au_{144}$  Cluster from Ab Initio TDDFT calculations.* H.-Ch. Weissker\*, H. Barrón, L. Fernández-Seivane, and X. López-Lozano\*.

May.28-31, 2013 International Conference Nanomeeting – 2013, Physics, Chemistry and Applications of Nanostructures, Minsk, Belarus.

**Talk:** *Optical Properties of Bimetallic Nanoalloys from TDDFT – Absorption Spectra of 13-Atom Noble Metal Clusters.* H.-Ch. Weissker\*, H. Barrón, L. Fernández-Seivane, and X. López-Lozano.

Apr.7-9, 2013 COST Action Meeting MP0903 NANOALLOY. Nanoalloys as Advanced Materials: From Structure to Properties and Applications. Workshop – Working groups 2 and 4. Domaine de Valpré, Lyon, France.

**Poster:** *Structure and Optical Response of 13-Atom Bimetallic Nanoalloys from Ab Initio TDDFT.* H.-Ch. Weissker\*, C. Mottet, H. Barrón, L. Fernández-Seivane, and X. López-Lozano.

– 2012 –

Dec.17-19, 2012 Réunion Plénière du GDR Nanoalliages, Orleans, France.

**Talk:** *Optical Response of Ag–Au Nanoalloys from Ab Initio TDDFT Calculations.* H.-Ch. Weissker\*, Christine Mottet, and X. López-Lozano.

Dec.11, 2012 Workshop on Nanostructures as Efficient Solar Energy Converters, Laboratoire PROMES, Perpignan, France.

**Talk:** *Surface Plasmon and Optical Response in Bimetallic Nanoalloys from Ab Initio TDDFT.* H.-Ch. Weissker\*. C. Mottet, H. Barrón, L. Fernández-Seivane, and X. López-Lozano.

Oct.5, 2012 2012 COS Research Conference. Physics & Astronomy and PREM Symposium. The University of Texas at San Antonio, San Antonio, TX, USA.

**Poster:** *Study of Structural Transitions – Electronic and Magnetic Properties of Ag/Au Nanoparticles.* H. Barrón\*, L. Fernández-Seivane, H.-Ch. Weissker and X. López-Lozano.

Jul.8-13, 2012 XVI ISSPIC, International Symposium on Small Particles and Inorganic Clusters. Katholieke Universiteit, Leuven, Belgium.

**Poster:** *Systematic Study of the Adsorption of Thiol Molecules on Noble-Metal Nanoparticles.* H. Barrón\*, F. Hidalgo, L. Fernández-Seivane, C. Noguez and X. López-Lozano.

**Poster:** *Composition and Structure of Small Noble-Metal Nanoalloys.* H. Barrón, J. O. Benson, L. Fernández-Seivane\*, H.-Ch. Weissker and X. López-Lozano.

**Poster:** *Surface Plasmon and Optical Response in Bi-metallic Nanoalloys from Ab Initio TDDFT Calculations.* H.-Ch. Weissker\*, H. Barrón, L. Fernández-Seivane, J. O. Benson, and X. López-Lozano.

Jul.4-6, 2012 Workshop: Theoretical Challenges in Electronic Structure of Clusters and Nanoparticles, CECAM-HQ-EPFL (École Polytechnique Fédérale de Lausanne); Lausanne, Switzerland.

**Poster:** *Structural Transitions in 13-Atom Ag/Au Nanoalloys.* H. Barrón, L. Fernández-Seivane\*, H.-Ch. Weissker and X. López-Lozano.

**Poster:** *Surface Plasmon and Optical Response in Ag-Au Nanoalloys from Ab Initio TDDFT Calculations.* H.-Ch. Weissker\*, H. Barrón, L. Fernández-Seivane, and X. López-Lozano.

Mar.22-24, 2012 2012 Spring Joint Meeting of the Texas Sections of the AAPT and APS and Zone 13 of the Society of Physics Students (TSAPS/AAPT/SPS), San Angelo State University, San Angelo, USA

**Talk:** *Systematic Study of the Adsorption of Thiol Molecules on Noble-Metal Nanoparticles.* H. Barrón\*, F. Hidalgo, L. Fernández-Seivane, C. Noguez and X. López-Lozano.

**Talk:** *Composition Dependence of the Properties of Noble-Metal Nanoalloys.* H. Barrón\*, L. Fernández-Seivane, J. O. Benson, H.-Ch. Weissker and X. López-Lozano.

**Talk:** *Spin Effects in Isolated Mono- and Bilayer Molybdenum Disulfide Nanowires.* L. Fernández-Seivane\* and X. López-Lozano.

– 2011 –

Nov.16-18, 2011 First Meeting of the American Initiative on Metal Clusters and Nanoalloys. The University of Texas at San Antonio, San Antonio, TX, USA.

**Talk:** *Ab Initio DFT Study of the Adsorption of Thiol Molecules on Au Nanoparticles.* H. Barrón\*, F. Hidalgo, L. Fernández-Seivane, C. Noguez, M. Olvera de la Cruz, Miguel José-Yacamán and X. López-Lozano\*.

Nov.07-10, 2011 International Symposium on Clusters and Nano-Structures (Energy, Environment, and Health), Richmond, Virginia, USA

**Poster:** *Ab Initio Study of Methyl-thiol Adsorption on Au Clusters.* H. Barrón\*, L. Fernández-Seivane, M. Olvera de la Cruz, Miguel José-Yacamán, and X. López-Lozano\*.

Oct.30, 2011 2011 COS Research Conference. The University of Texas at San Antonio, San Antonio, TX, USA.

**Poster:** *Ab Initio DFT Study of the Adsorption of Thiol Molecules on Au Nanoparticles.* H. Barrón\*, L. Fernández-Seivane, M. Olvera de la Cruz, Miguel José-Yacamán, and X. López-Lozano.

Oct.06-08, 2011 2011 Fall Joint Meeting of the Texas Sections of the AAPT and APS and Zone 13 of the Society of Physics Students (TSAPS/AAPT/SPS), Texas A&M University-Commerce, Commerce Texas, USA

**Talk:** *Ab Initio DFT Study of the Adsorption of Thiol Molecules on Au Nanoparticles.* H. Barrón\*, L. Fernández-Seivane, M. Olvera de la Cruz, Miguel José-Yacamán, and X. López-Lozano.

Sep.27-30, 2011 16th ETSF Workshop on Electronic Excitations. Turin, Italy.

**Talk:** *Influence of (Semi-)Core Electron Polarization on Electron Energy-Loss Spectra.*



H.-Ch. Weissker\*, M. Cazzaniga, L. Caramella, E. Luppi, X. López-Lozano, G. Onida, and L. Reining.

Jun.27-30, 2011 Réunion Générale du GDR coDFT, Obernai, France.  
**Talk:** *Optical Properties of Pure and Core-Shell Noble-Metal Nanoalloys from TDDFT.* H.-Ch. Weissker\*, Christine Mottet, and X. López-Lozano.

– 2010 –

Oct.19-24, 2010 XV ISSPIC, Oaxaca, Mexico.  
**Poster:** *DFT Study of the Enantiospecific Adsorption on Au<sub>55</sub> Clusters.* X. López-Lozano\*, L. A. Pérez, and I. L. Garzon

May.28, 2010 2010 COS Research Conference. University of Texas at San Antonio, San Antonio, TX, USA.  
**Talk:** *DFT Study of MoS<sub>2</sub> Nanowires.* X. López-Lozano\*, S. Botti, M. A. L. Marques, S. Mejia, Miguel José-Yacamán, A. Rubio.

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– 2001 - 2008 –

Oct.23-27, 2008 13th ETSF/Nanoquanta Conference - Theoretical Spectroscopy and Quantum Transport, Pugnochiuso, Vieste, Italy.  
**Poster:** *Plasmon Excitation of Single-Walled Carbon Nanotubes*

Jun.9-12 2008 Workshop: Structural, Electronic and Transport Properties of Quantum Wires, CECAM-ENS; Lyon, France.  
**Poster:** *Electronic and Catalytic Properties of MoS<sub>2</sub> Nanowires*

May.19-23, 2008 5th Nanoquanta Young Researchers' Meeting, Modena, Italy.  
**Poster:** *Optical Properties of Carbon nanotubes: A Study of the Momentum-Transfer Dependence*

May.14-16, 2008 JEELS 2008: Journées de EELS 2008; Poitiers, France.  
**Poster:** *The Momentum-Transfer-Dependent Optical Response of Single-Walled Carbon Nanotubes*

Apr.03, 2008 Réunion thématique IRAMIS (Institut Rayonnement Matière Saclay), Structure électronique et Modélisation atomistique, CEA (Commissariat à l'Énergie Atomique) Saclay, France.  
**Poster:** *Electronic and Catalytic Properties of MoS<sub>2</sub> Nanoplatelets: An Ab Initio Study*

Dec.3-4, 2007 Workshop on Electrons in Graphene, LPSO (Laboratoire de Physique des Solides, Orsay), Orsay, île de France, France.  
**Poster:** *Ab initio Study of the Wave-Vector-Dependence on the Optical Response of Small Carbon Nanotubes*

Oct.18-22, 2007 12th Nanoquanta Workshop 2007, Aussois, Savoy, France.  
**Poster:** *Wave-vector-Dependence Study of the Dielectric and Energy-Loss Functions of Small Carbon Nanotubes*

May.15-18, 2007 4th Nanoquanta Young Researchers' Meeting, Donostia-San Sebastián, Basque Country, Spain.  
**Poster:** *Electronic and Catalytic Properties of MoS<sub>2</sub> Nanoplatelets*

- Mar.27-30, 2007 Réunion Générale du GDR DFT++, Résidence L'Escandille, Autrans (Isère), France.  
**Poster:** *Enantiospecific Adsorption of Chiral Molecules on Chiral Au Clusters.*
- Mar.5-9, 2007 APS March Meeting 2007, Denver CO, USA.  
**Talk:** *Enantiospecific Adsorption of Chiral Molecules on Chiral Au Clusters.*
- May.2-4.05, 2006 1st Mexican Workshop on Nanostructured Materials, Puebla, Pue., Mexico.  
**Poster:** *Enantiospecific Adsorption on Chiral Au<sub>55</sub> clusters.*
- Mar.13-17, 2006 APS March Meeting 2006, Baltimore MD, USA.  
**Talk:** *Enantiospecific Adsorption on Chiral Gold Nanoclusters from DFT Calculations.*
- Jul.03-08, 2005 ICFSI-10: 10th International Conference on the Formation of Semiconductor Interfaces, Aix-en-Provence, France.  
**Talk:** *Theoretical Studies of Atomic, Electronic and Spin Properties of Quasi-1D In/Si(111) Systems.*
- May23-25, 2005 IUPAP 2nd International Conference of Women in Physics, Rio de Janeiro, Brasil.  
**Poster:** *Women in Physics: the mexican working group.*
- Nov.17-19, 2004 Conference: Latin American Women in Exact and Life Sciences, Rio de Janeiro, Brasil. **Poster:**
- Oct.25-29, 2004 XLVII Congreso Nacional de Física, Sonora, Hermosillo, Mexico. **Poster.**
- Jul.18-21, 2004 VIII-ECSCD: 8th European Conference on Surface Crystallography and Dynamics, Segovia, Spain. **Poster.**
- Mar.8-12, 2004 Frühjahrstagung der Deutschen Physikalischen Gesellschaft, Regensburg, Germany. **Poster.**
- Jun.8-18, 2003 PASI-2003: Panamerican Advanced Studies on Physics at the Nanometer Scale, Bariloche, Argentina. **Poster.**
- May.26-30, 2003 OSI-V: 5th International Conference of Optics of Surfaces and Interfaces, León, Gto., Mexico. **Talk.**
- Dec.2-05, 2002 XVI-SLAFES: Simposio Latinoamericano de Física del Estado Sólido, Mérida, Venezuela. **Poster.**
- Oct.28-Nov.1, 2002 XLV Congreso Nacional de Física, León, Gto., Mexico. **Poster.**
- Sep.30-Oct.4, 2002 XXII Congreso Nacional de la Sociedad Mexicana de Ciencia de Superficies y Vacío, Veracruz, Mexico. **Poster.**
- Jun.6-7, 2002 VIII Encuentro Regional de Investigación y Enseñanza de la Física, Puebla, Pue., Mexico. **Poster.**
- May.13-15, 2002 V Taller de Estudiantes de Posgrado, Puebla, Pue., Mexico. **Poster.**
- 07.03.-0.9.03, 2002 IUPAP 1st International Conference on Women in Physics, UNESCO, Paris, France. **Poster.**
- Oct.30-Sep.3, 2000 XLIII Congreso Nacional de Física, Puebla, Pue., Mexico. **Talk.**
- Jun.18-Jul.6, 2001 XXXIII-ELAF: Escuela Latinoamericana de Física, Colegio Nacional, Mexico City, Mexico.  
**Talk:** *Classical Dynamics in a Coulomb + Harmonic Potential.*

## B. INVITED TALKS 2009 – 2014

Invited Conference Talks: 7

Other Invited Talks: 5

Total Invited Talks since 2004: 16

\* – Presenter

– 2014 –

Aug.17-21, 2014 *Discovering the Properties of Exotic MoS<sub>2</sub> Nanostructures*. X. López-Lozano\*  
XXIII IMRC (International Material Research Congress), Symposium 6A: Advanced Catalytic Materials. Materials Research Society, Cancun, Mexico.

Apr.10, 2014 *Gold and Silver Nanoparticles: Structure and Optical Response*. X. López-Lozano\*.  
Spring Seminar Series of the School of Physics of the Meritorious Autonomous University of Puebla (FCFM-BUAP), Puebla, Pue., Mexico.

– 2013 –

Apr.7-9, 2013 *Surface Plasmon and Optical Response in Bimetallic Nanoalloys from an Ab Initio TDDFT*. H.-Ch. Weissker, Christine Mottet, H. Barrón, L. Fernández-Seivane, and X. López-Lozano\*.  
COST Action Meeting MP0903 NANOALLOY. Nanoalloys as Advanced Materials: From Structure to Properties and Applications. Workshop – Working groups 2 and 4. Domaine de Valpré, Lyon, France.

– 2012 –

Nov.28, 2012 *Carbon Nanotubes. A Hands-On Activity*. H. Barrón\*, L. Fernández-Seivane, and X. López-Lozano\*. 2012 Fall Seminar Series on Nanotechnology, Northwest Vista College, San Antonio, TX, USA.

Oct.5, 2012 *Structural Properties and Spin Effects of Flat, Twisted and Helical MoS<sub>2</sub> Nanostructures*. H. Barrón, L. Fernández-Seivane\*, and X. López-Lozano.  
2012 COS (College of Sciences) Research Conference. Physics & Astronomy and PREM Symposium. The University of Texas at San Antonio, San Antonio, TX, USA.

Apr.20, 2012 *The Practical Applications of Carbon Nanotubes + Hands-On Activity: Building A Carbon Nanotube*. X. López-Lozano\*. 2012 Spring Seminar Series on Nanotechnology, Northwest Vista College, San Antonio, TX, USA.

– 2011 –

Sep.21-24, 2011 *The Molecular Selectivity of Au Nanoparticles: An Ab Initio Study*. H. Barrón, L. Fernández-Seivane, I. L. Garzón, L. A. Pérez, H.-Ch. Weissker, and X. López-Lozano\*.  
NSBP/NSHP (National Society of Black Physicists and the National Society of Hispanic Physicists) Joint Conference, Austin, TX, USA.

Aug.14-19, 2011 *Atomic and Electronic Properties of Quasi-One Dimensional MoS<sub>2</sub> Nanowires*. X. López-Lozano\*, S. Botti, M. A. L. Marques, S. Mejia, Miguel José-Yacamán, A. Rubio.

XX IMRC, Symposium: Nanostructured Materials and Nanotechnology. Materials Research Society, Cancun, Mexico.

– 2010 –

Oct.29, 2010 Invited participant for the *Managing Work/Life* Panel. X. López-Lozano\*. SHPE 2010 (Society of Hispanic Professional Engineers) Conference, Cincinnati, OH, USA.

Mar.29, 2010 *A Potential Application of Gold Nanoclusters*. X. López-Lozano\*. 2010 Spring Seminar Series on Nanotechnology, Northwest Vista College, San Antonio, TX, USA.

– 2009 –

Oct.15-18, 2009 *Optical Properties of Low-Dimensional Systems*. X. López-Lozano\*. 2009 SACNAS (Society for Advancement of Chicanos and Native Americans in Science ) National Conference, Dallas, TX, USA.

Aug.20, 2009 *DFT Study of the Cysteine Adsorption on Au<sub>55</sub> Clusters*. L. A. Pérez, X. López-Lozano\* and I. L. Garzon  
ACS (American Chemistry Society) 238th National Meeting, Washington D.C., USA.

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– 2004 - 2008 –

Nov.17, 2008 *Propiedades Estructurales y Electrónicas de Nanoalambres de MoS<sub>2</sub>*. X. López-Lozano\*. Centro de Investigación, Innovación y Desarrollo en Ingeniería y Tecnología. (CIDIT), Monterrey, Nuevo León, Mexico.

Nov.10, 2008 *Respuesta Óptica de Nanotubos de Carbono de Pared Monoatómica*. X. López-Lozano\*. Internal Conference Cycle of REGINA (Red de Grupos de Investigación en Nanociencia) at the National Autonomous University of Mexico (IF-UNAM).  
[www.fisica.unam.mx/nanoifunam/index-en.htm](http://www.fisica.unam.mx/nanoifunam/index-en.htm)

Nov.07, 2008 *Optical Response of Single-Walled Nanotubes: An Ab Initio Study of the Momentum-Transfer-Dependence*. X. López-Lozano\*. Department of Physics and Astronomy, University of Texas, San Antonio, TX, USA.

Sep.1, 2004 *Propiedades Estructurales y Electrónicas de Nanoalambres de In sobre Si(111)*. X. López-Lozano\*. Internal Conference Cycle of REGINA, IF-UNAM, Mexico.

## SCHOOLS, WORKSHOPS AND SPECIALIZED COURSES

A. – 2009 - 2014 – Summary

Grant-Applications-Related	Research-Related	Teaching-Related	Total
3	2	4	9

– Grant Applications-Related –

Sep.19, 2013 *Proposal Development and Navigating Federal Granting Agencies* by Dr. Bernard Arulanandam, Assistant Vice President for Research Support, Faculty Center, 1604 Campus, The University of Texas at San Antonio, San Antonio, TX, USA.

May.16, 2011 *Write Winning Grants Seminar & Workshop* by David C. Morrison, Ph.D., The University of Texas at San Antonio, San Antonio, TX, USA.

Nov.11, 2010 NSF Workshop, AET 0.212, 1604 Campus, The University of Texas at San Antonio, San Antonio, TX, USA.

– Research-Related –

Aug.01-05, 2011 Summer Supercomputing Institute 2011. Texas Advanced Computing Center (TACC), Austin, TX, USA.

Jun.07-10, 2010 Efficient Density-Functional Calculations with Atomic Orbitals: A Hands-On Tutorial on the SIESTA Code. The Faculty of Sciences at University of Cantabria, Santander, Spain.

– Teaching-Related –

May.15-17, 2013 *The 2013 Provosts Academy on Critical Thinking*. Teaching & Learning Center, 1604 Campus, The University of Texas at San Antonio, San Antonio, TX, USA.

Nov.14, 2012 Training class for Blackboard Learn 9.1: Bronze Level. Faculty Instructional Technology Lab, 1604 Campus, The University of Texas at San Antonio, San Antonio, TX, USA.

Sep.14, 2012 *Six Checkpoints for Motivation in Learning Workshop* by Marilla Svinicki, Ph.D., Teaching & Learning Center, 1604 Campus, The University of Texas at San Antonio, San Antonio, TX, USA.

Nov.12-15, 2009 November New Physics and Astronomy Faculty Workshop, AAPT (American Association of Physics Teachers), American Center for Physics, College Park, MD, USA.

## B. Earlier Schools, Workshops and Specialized Courses.

– 1998 - 2008 –

- Feb.11-15, 2008 Basic Techniques and Tools for Development of Atomic-Scale Software, CECAM (Centre Européen de Calcul Atomique et Moléculaire), Lyon, France.
- Dec.10-14, 2007 Theoretical Spectroscopy Lectures: Theory and Codes, CECAM, Lyon, France.
- Dec.4-6, 2007 Programming language FORTRAN 95-2, I.D.R.I.S. (Institut du Développement et des Ressources en Informatique Scientifique), Orsay Cedex, France.
- Oct.9-11, 2007 Programming language FORTRAN 95-1, I.D.R.I.S., Orsay Cedex, France.
- Jan.29-31, 2007 MPI-1 (Message Passing Interface), I.D.R.I.S., Orsay Cedex, France.
- 30.09.-04.10, 2002 Short Course: *Materials Characterization*, by Richar Brundle, Director of Defect and Thin-Film Characterization Laboratory, Applied Materials, California, EUA. XXII Congreso Nacional de la Sociedad Mexicana de Ciencia de Superficies y Vacío, Veracruz, Mexico
- Jul.12-24, 1998 VII Summer School in Physics: *The Molecular View of Matter*, Cuernavaca Morelos, Mexico.

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## GRANTING ACTIVITIES

### Summary of Grant Applications during 2009 – 2014

Total Number of Applications: 14

Total Number Granted: 2

In Preparation: 2

Total Number of Granted Applications for Computational Time: 2

Grant Type	Agency	Award Amount	Award Period	Affiliation
External	NSF DMR-1103730	\$344,063	Jan. 2011 – Jan. 2013	Co-PI
Internal	UTSA-TRAC FY2011-2012	\$22,000	Sep. 2011 – Sep. 2012	PI
External	NSF PREM DMR-0934218	\$2.7M	Sep. 2009 – Sep. 2014	Participant

Grant Applications submitted for Computational Time at the Texas Advanced Computing Center (TACC).

Projects Type: Research; Field of Science: Materials Research (DMR); Affiliation: PI;

Award Period: SP 2011– FL 2012.

Project Title	Unix Group	Project Charge Code	Compute Award	Storage Award	Students
<i>Ab Initio</i> Study of Nanoparticles	G-803370	Au-Thiol_DFT_Study	650879 SUs	1024 GBs	2 Graduate 1 Postdoc
Systematic Design of Novel Molybdenum-Disulfide Nanocatalysts	G-803371	MoS2_Nanocatalysts	217000 SUs	1024 GBs	1 Graduate 1 Postdoc

— 2013–2014 —

Project/Proposal Title	Agency	Award Amount	Award Period	Affiliation
“CAREER” — Faculty Early Career Development	NSF	In preparation	[Sep. 2015 – Aug. 2018]	PI
Plasmon Emergence Phenomena in Ligand-Protected Noble-Metal Nanoparticles	Air Force Office of Scientific Research (AFOSR)	\$200,000-\$400,000 In Preparation	5 years	PI
— Designing the Optical Response of Ligand-Protected Nobel-Metal Nanoparticles — Plasmon Emergence Phenomena	NSF CHEM Division	Unfunded	[Sep. 2014 – Aug. 2017]	PI
Designing the Optical Response of Nobel-Metal Nanoparticles	Welch Foundation	Unfunded	[Jun. 2015 – May 2018]	PI
Pre-Proposal Title: Study and Design of the Optical Properties of Nobel-Metal Nanoparticles	Norman Hackerman Advance Research Program 2013 (NHARP-2013)	Not Approved	Two-Years	PI

— 2012 —

Project/Proposal Title	Agency	Award Amount	Award Period	Affiliation
Optical properties of Nanoalloys: Size and Chemical Mixture Effect	Welch Foundation	Unfunded	[Jun. 2013 – May. 2018]	PI
Tuning the Optical Response of Intermediate Size Nanoparticles using Small Nanoalloys as Building Blocks.	Research Corporation for Science Advancement Cottrell Scholar Award	Unfunded	[May 2012 – May 2015]	PI
REU site: Physics at UTSA/SwRI: Materials and Astrophysics, and Space Physics	NSF	Unfunded	[May 2013 – Apr. 2016]	Participant
IGERT-TSM: Nanoparticles and Low Dimensional Systems Synthesis, Characterization, Applications in Biology, Medicine and the Environment	NSF	Unfunded	[May 2013 – Apr. 2018]	Participant

— 2009 – 2011 —

Project/Proposal Title	Agency	Award Amount	Award Period	Affiliation
Designing Novel MoS <sub>2</sub> Nanocatalysts	UTSA	\$22,000	[Sep. 2011 – Sep. 2012]	PI
Oxide and Metal Nanoparticles Alloys at the Nanoscale; The Case of Nanoparticles. Second Phase.	NSF	\$344,063	[Jan. 2011 – Jan. 2013]	Co-PI
Oxide and Metal Nanoparticles: The Interface between Life Sciences and Physical Sciences	NSF	\$2.7M	[Sep. 2009 – Sep. 2014]	Participant
Systematic Design of Novel Molybdenum-disulfide Nanocatalysts	NSF	Unfunded	[May. 2012 – May. 2015]	PI
IGERT-TSM Tunable Sensing Materials through Multiscale Synthesis, Multiwavelength Actuating, and Multiphysics Design.	NSF	Unfunded	[May. 2011 – Apr. 2016]	Participant
Center for Microsystems and Nanotechnology Education	DoD	Unfunded	[Mar. 2011 – Feb. 2016]	Co-PI
REU site: Physics, Astrophysics and Space Physics at UTSA and SwRI	NSF	Unfunded	[May 2010 – Apr. 2013]	Participant
REU site: Physics, Astrophysics and Space Physics at UTSA and SwRI	NSF	Unfunded	[May 2009 – Apr. 2012]	Participant

**Grant-Related Activities during 2009 – 2014:**

- Spring 2013 Visits to the NSF and DARPA to explore the possibilities of funding, meet the program managers and receive feedback to my whitepapers.
- Fall 2011 A visit to the NSF to explore the possibilities of funding, meet the program managers and receive feedback to my whitepapers.
- 2010 - 2011 I've been in charge of measuring the impact of the outreach program of the NSF-PREM grant with the Nanotechnology Seminar Series at the Northwest Vista community College.
- Fall 2010 Organization, with other junior faculty members in the department (Dr. Lopez-Lozano, Dr. Marucho, Dr. Nash and Dr. Peralta) into a Proposal Writing Work Group.
- May.16, 2011 I attended the *Write Winning Grants Seminar & Workshop* given by David C. Morrison, Ph.D., The University of Texas at San Antonio, San Antonio, TX, USA.



## TEACHING ACTIVITIES

List of courses taught 2009–2014 at the University of Texas at San Antonio, San Antonio, TX, USA.

Lower Division	Upper Division	Graduate Level	Total
10	4	2	16

  

Semester	Course Prefix & Nr.	Course Title	Course Level
FL 2014	PHY 3203	Classical Mechanics I	UD
SP 2014	PHY 1603	Algebra-Based Physics I	LD
FL 2013	PHY 7603	Nanostructures: Theo & Simul	GR
FL 2013	PHY 1603	Algebra-Based Physics I	LD
SP 2013	PHY 1603	Algebra-Based Physics I	LD
SP 2013	PHY 1603	Algebra-Based Physics I	LD
FL 2012	PHY 1603	Algebra-Based Physics I	LD
FL 2012	PHY 1603	Algebra-Based Physics I	LD
SP 2012	PHY 1603	Algebra-Based Physics I	LD
SP 2012	PHY 1603	Algebra-Based Physics I	LD
FL 2011	PHY 7603	Nanostructures: Theo & Simul ( <b>New</b> )	GR
FL 2011	PHY 3203	Classical Mechanics I	UD
SP 2011	PHY 1943	Physics for Scientists I	UD
FL 2010	PHY 3203	Classical Mechanics I	UD
FL 2010	PHY 1943	Physics for Scientists I	LD
SP 2010	PHY 1943	Physics for Scientists I	LD
FL 2009	PHY 3203	Classical Mechanics I	UD

Acronyms:: SP: Spring; FL: Fall; LD: Lower Division; UD: Upper Division; GR: Graduate Level

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Aug.1., 2005–Jan.11, 2006. Informal lectures of *Solid State Physics* to Master level students and partial direction of a PhD student at the IF-UNAM in Mexico city.

Teaching-assistantship of Theoretical Physics at the IFUAP-BUAP, Puebla, Pue., Mexico.

Date	Course Title	Course Level
Feb.–May., 2003	Electromagnetism	Pre-Master
Aug.–Dec., 2001	Electrodynamics	Master
May.–Jul., 2001	Modern Physics	Pre-Master
Jan.–May., 2001	Statistical Physics	Master

### General Teaching-Related Activities:

– 2014 –

- Dr. Fernando Mendoza Santoyo, visiting professor, was asked to attend my class to get his comments and recommendations to keep improving my teaching.
- Meetings with Dr. Rafael López-Mobilia were set to continue getting his advice on how to improve my teaching.

– 2013 –

- Useful meetings with Dr. Rafael López-Mobilia and Dr. Eric Schlegel were continued to get advice on how to improve my teaching after they attended my classes.

- As required by the Dean George Perry, I attended the 2013 Provosts Academy on Critical Thinking on May 15-17, 2013.

– 2012 –

- Useful meetings with Dr. Rafael López-Mobilia and Barbara Millis were set up to get advice on how to improve my teaching.
- I attended the workshop: Six Checkpoints for Motivation in Learning, at the Teaching & Learning Center here at UTSA.
- The Hands-On Activity of Carbon Nanotubes, originally designed for high school students, was integrated formally as part of the Seminar Series on Nanotechnology at Northwest Vista College, San Antonio, TX.

During the Spring and Fall, my Phd student and my Postdoc were involved in this activity. The goal has been to teach community college students how to build manually a model of a nanostructure like a carbon nanotube and learn about its different applications.

– 2009 - 2011 –

- Nov. 2009: attended the *New Physics and Astronomy Faculty Workshop* organized by the AAPT (American Association of Physics Teachers);
- Prepared and developed the educational material of four (4) courses;
- Fall 2010 and Spring 2011: responsible to collect the data for SACS (Southern Association of Colleges and Schools) evaluation of the Natural Science Domain of PHY 1943 for its accreditation;
- For PHY 3203, I developed extra course material that covers Vector Calculus and Differential Equations to compensate for shortcomings in students' background;
- Fall of 2011: I developed the new graduate course PHY 7603 “Special Topics in Physics: Nanostructures: Theory & Simulation.” which introduces state-of-the-art theory of ab initio calculations together with hands-on sessions.
- Summer 2010: an instructional-related grant application was submitted to the DOD (Department of Defense) but was not funded.
- I developed instructional material for high-school students to help them to get familiar with the structure and properties of carbon nanotubes using atomic models for visualization; the material was used in the “Nanotechnology Seminar Series”.

## List of Students Mentored in Research Activities.

Undergraduate: 2 (Summer Programs)

Graduate: 1 (PhD student )

Graduate: 2 (Supervised Graduate Students)

Postdocs: 1

NVC Community College Student: 1 (Internship)

– 2014 –

**Arturo Alejandro Canales Benavides**, undergraduate student, 2014 summer stay within the framework of the UTSA Research Immersion for Monterrey Tec Undergraduates.

**Andres Delgado**, undergraduate student, 2014 summer stay within the framework of Louis Stokes Alliances for Minority Participation Program (LSAMP).

**Shaylynn Clark**, graduate student, volunteered to work in my lab for the Summer 2014 and started training in computational Density Functional Theory and visualization software programs.

**William Ernest Barnes**, Community College student, started his mandatory Internship required by the Nanotechnology Program of Northwest Vista College during the Spring 2014. The student did not conclude for personal reasons.

– 2013 –

**Hector Barron Escobar**, Ph.D. Student since May of 2011 was funded from the NSF-PREM grant DMR-0934218.

**Topic:** *Structural and Electronic Properties of Thiol Molecules on Au Clusters and Bimetallic Nanoparticles*

On May 29th of 2012, this student presented his **Oral Qualifying Exam** and successfully advanced to the PhD candidacy.

**Talk:** *Electronic, Magnetic and Optical Properties of Bimetallic Nanoparticles*

**The PhD student Hector Barrón graduated on July 2013.** Following his graduation, he got a **Postdoctoral Fellowship in the Modeling of Nanocatalysts**, with CSIRO Materials Science and Engineering in the group of Dr. Amanda Barnard in Australia.

**Angela Bolineau**, graduate student, volunteered to work in my lab in the fall of 2013 and started training in computational Density Functional Theory in order to create a collaboration with Dr. Chonglin Chen at UTSA.

– 2012 –

**James O. Benson**, was a Ph.D. Student who joined my group on December 2012. A DoE (Department of Energy) fellowship application was submitted on Jan. 04, 2012 for funding. Proposes research topic: *Optical and Electronic Properties of Supported Metal Nanoparticles for Plasmonic Solar Cells from Ab Initio Calculations.* The student abandoned the Physics Program for personal reasons.

## Other people under my supervision

– Sep.2011 - Mar.2013 –

**Lucas Fernández Seivane**, Postdoctoral Fellow funded with my start-up package.  
Topic: *Ab Initio Simulations of the Properties of MoS<sub>2</sub> Nanostructures and Bimetallic Nanoparticles.*

## PhD Student Fellowships, Awards and Student Scholarship Applications:

– 2012 - 2013–

- My PhD student Hector Barron graduated on July 2013 and was granted the following scholarships and funding from different organizations:
    - Following his graduation, a Postdoctoral Fellowship in the Modeling of Nanocatalysts, with CSIRO Materials Science and Engineering in the group of Dr. Amanda Barnard in Australia.
    - COS Doctoral Student Fellowship Award 2012-2013. Granted by The University of Texas at San Antonio, TX, USA. on Dec.11<sup>th</sup>, 2012.
    - Funding to attend the Society for Advancement of Chicanos and Native Americans in Science (SACNAS) annual meeting, Oct.11-14, 2012, Seattle, WA, USA. NSF-PREM grant DMR-0934218.
    - National Science Foundation Travel Award Winner 2012. This funding was granted to Hector Barron to attend the CAMd (Center for Atomic-Scale Material Design) Summer School 2012 in Electronic Structure Theory and Materials Design, Aug.11-17, 2012, Lyngby, Denmark.
  - Spring 2012. PhD student J. O. Benson applied together with me to the Department of Energy Graduate Fellowship program for a PhD scholarship. Unfunded.
  - My postdoc, Dr. Lucas Fernández Seivane, was granted a National Science Foundation Travel Award 2012 to attend the Workshop: Theoretical Challenges in Electronic Structure of Clusters and Nanoparticles at the CECAM-HQ-EPFL in Lausanne, Switzerland, to present the results of our research.
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## SERVICE ACTIVITIES

### A. Summary of Permanent and Quasi-Permanent Service Activities:

Program	Role	Date	Organization
1. Organizing Committee of The College of Science (COS) Research Conference	<b>Member</b>	FL 2013	COS, UTSA
		FL 2013	COS, UTSA
		FL 2012	
		SP 2010	
	Physics & Astronomy Session		
	<b>Chairman</b>	Oct. 18 <sup>th</sup> , 2013	
	Physics & Astronomy Session and PREM Symposium		
	<b>Chairman</b>	Oct. 5 <sup>th</sup> , 2012	
	Physics & Astronomy Session		
	<b>Chairman</b>	May. 28 <sup>th</sup> , 2010	
	Physics & Astronomy Poster Session		
	<b>Judge</b>	Oct. 5 <sup>th</sup> , 2012	
	Physics & Astronomy Poster Session		
	<b>Judge</b>	Oct. 30 <sup>th</sup> , 2011	
2. – Nanotechnology Seminar Series – at Northwest Vista Community College in San Antonio	<b>Organizer</b> Total Talks Organized: ~ 45	SP 2014	UTSA
		FL 2013	COS
		SP 2013	Department
		FL 2012	
		SP 2012	
		FL 2011	
		SP 2011	
		FL 2010	
		SP 2010	
3. Recruitment Committee (Graduate Students)	<b>Member</b> Presentation of the Physics Program at UTSA in several Conferences that I attended.	SP 2010 – SP 2014	Department
4. Department's Website and Brochure	<b>Collector</b> for Research-related figures and pictures of Faculty	FL 2009 – SP 2010	Department
5. Qualifying Examination and Dissertation Committee	<b>Member</b> Students: Hector Barron - Qualifying Exam - - Dissertation - Samantha Franklin - Dissertation - Shanna Pahl - Qualifying Exam -		Department
		May, 2012	
		July, 2013	
		TBD	
		TBD	

## SERVICE ACTIVITIES [Continued]

B. Summary of Service Activities performed as an active Participant of the internal NSF-PREM DMR-0934218 grant - Spring 2011 – Summer 2014 -

Program	Role	Date	Organization
1. Educational and Outreach	Sub-Committee <b>Member</b>	SP 2011 – FL 2013	COS, UTSA
2. NSF Site Visits of – External Advisory Committee –	Research Presentation: <i>Poster</i> NSF Site Visit Rehearsal Educational and Outreach Activities Presentation: <i>Talk</i> Research Presentation: <i>Poster</i>	Feb. 18 <sup>th</sup> , 2011 Oct. 7 <sup>th</sup> , 2011 Oct. 13 <sup>th</sup> -14 <sup>th</sup> , 2011	
	Research Highlights provided for Annual PREM Reports: 3		
3. NANODay	Organizing Committee <b>Member</b>	SP 2011 – FL 2013	
	“Carbon Nanotubes” Activity <b>Creator</b> Developed Material: –Atomic Models ; –A Power Point Presentation; –A short Instructional Manual for Atomic Structure Software usage	SP 2011	
	– NanoDay at UTSA – “Carbon Nanotubes” Activity New Material Added: – 5 <i>Instructional Posters</i> 3rd Annual CORE4 STEM Expo – NanoDay at UTSA –	Feb. 21 <sup>th</sup> , 2011 Jun. 20 <sup>th</sup> , 2011 Apr. 6 <sup>th</sup> , 2012 Nov. 10 <sup>th</sup> , 2012 Mar. 3 <sup>th</sup> , 2013	NSF-PREM Educational and Outreach Program
4. Mobile NANODay	4th Annual CORE4 STEM Expo <i>Henry B. Gonzalez</i> Convention Center in San Antonio, TX, US	Nov.13 <sup>th</sup> -14 <sup>th</sup> , 2013	
5. Measuring the impact of the – Nanotechnology Seminar Series – at Northwest Vista College for the NSF-PREM Outreach Program	Questionnaire <b>Developer</b>  <b>Responsible</b> of Data Collection and Statistical Analysis	SP 2010 – SP 2012	
6. Collaboration Northwestern University (NU)	Efforts to promote and establish collaborative research among NSF-PREM Partner Institutions – UTSA - NU –	SP 2011 – SP 2013	

## SERVICE ACTIVITIES [Continued]

C. Miscellaneous Service Activities including One-Time Activity Services Performed

–2009 - 2014–

Program	Role	Date	Organization
1. <b>SACS</b> (Southern Association of Colleges and Schools) evaluation (of the Natural Science Domain) of PHY 1943 course for its <b>Accreditation</b>	<b>Responsible</b> of Data Collection and Statistical Analysis	SP 2011 FL 2010	UTSA
2. Sponsored by – ICNAM – International Center for Nanotechnology and Advanced Materials	Talk at the FCFM-BUAP, Mexico in support of UTSA's initiative to increase collaborations with Latin America	Apr. 10 <sup>th</sup> , 2014	COS, UTSA
3. Commencement Ceremony	<b>PhD Advisor</b>	Dec. 21 <sup>th</sup> , 2013	COS, UTSA
4. Commencement Ceremony	College of Sciences <b>Marshal</b>	Dec. 16 <sup>th</sup> , 2010	COS, UTSA
5. Nanotechnology Program Northwest Vista College	Nanotechnology Advisory Committee <b>Member</b>	FL 2010 – Present – Jun. 28 <sup>th</sup> , 2012 Dec. 03 <sup>th</sup> , 2010	Department
– Research-Related –			
6. COST Action Meeting MP0903 NANOALLOY Workshop – Working groups 2 and 4 Lyon, France	Oral Session <b>Chairman</b>	Apr. 09 <sup>th</sup> , 2013	
7. 2010 Joint Fall Meeting Texas Sections of the AAPT and APS and Zone 13 of the SPS at UTSA	Oral Session SM3 Nanoscience <b>Moderator</b> Poster Session FP1 <b>Judge</b>	Oct.21 <sup>th</sup> -23 <sup>th</sup> , 2010	

## SERVICE ACTIVITIES [Continued]

### D. Infrastructure Development Activities at UTSA.

Spring 2011 Using funds from my Start-Up Package, **I contributed to the development of the COS infrastructure** at UTSA. Specifically, I donated a M910 Blade Server (IXeon 2.26GHz, 146GB) to the High Performance Computing cluster Cheetah of the Center/Computational Biology Initiative (CBI). The goals of the CBI are to build infrastructure and foster the use of state-of-the-art core computational and analytic facilities, to enhance local expertise and significantly advance collaborative interdisciplinary bioscience research in San Antonio.

Nov.2009 – Fall 2011 In order to be able to develop a computational facility in the department, **I was in charge of setting up 4 (four) Computational Laboratories**, mine included, **and a Server Room**. The setting up of the computational labs started from scratch –shell space– with the designing of the electrical installation, the network and ventilation system, the furniture plans, etc.

Nov.2009 – Jun.2010 I held multiple meetings with the chairman of our department, the building's architect Rick Zamora, Jonathan Jarrell, as well as with Tech Support people, etc. until a balance between needs and budget was reached and a work order was submitted to set up (4) four computational laboratories and a server room.

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### E. Referee of Peer-Reviewed Journals

- Nanoscale
- ACSNano
- Journal of Physical Chemistry C
- The European Physical Journal D