

## **PEDRO A. DEROSA**

Associate Professor of Physics

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Grambling, LA 71245  
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### **EDUCATION**

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**Ph.D. in Physics** - December 5, 1997

National University of Córdoba-Faculty of Mathematics, Astronomy and Physics\*, Dept. of Physics - Córdoba, Argentina

Dissertation: "X-ray polarization from the interior of a cylinder, calculations, experiments and simulations". Advisor: Dr. Raúl T. Mainardi.

**"Licenciado" in Physics** (Equivalent to a B.S. plus a M.S. in physics\*\*) - March 14, 1993

National University of Córdoba-Faculty of Mathematics, Astronomy and Physics\*, Dept. of Physics - Córdoba, Argentina

Thesis: "Design of an Experiment in X-ray Fluorescence with Polarization", Advisor: Dr. Raúl T. Mainardi.

### **PROFESIONAL EXPERIENCE**

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2010-current:

**Grambling State University-Louisiana Tech University**

ASSOCIATE PROFESSOR

Joint Faculty Appointment between the Department of Physics at Grambling State University and the Institute for Micromanufacturing and the Physics Program at Louisiana Tech University.

2004-2010:

**Grambling State University-Louisiana Tech University**

ASSISTANT PROFESSOR

Joint Faculty Appointment between the Department of Physics at Grambling State University and the Institute for Micromanufacturing and the Physics Program at Louisiana Tech University.

2003-2004

**Louisiana Tech University, Ruston, LA**

**Institute for Micromanufacturing/Physics Program** (*September 2003-October 2004*)

RESEARCH ASSOCIATE

Conducted research, supervise graduates and undergraduate students, and teach undergraduate and graduate courses.

1998-2003:

**University of South Carolina, Columbia, SC**

**Dept. of Electrical Engineering** (*August 2001-August 2003*)

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\* Center of Excellence in Teaching and Research of the Third World Academy of Sciences, since 1994

\*\* Certified by "International Education Evaluation, Inc.", Charlotte, North Carolina

**Dept. of Chemistry and Biochemistry (November 1999-August 2001)**  
POSTDOCTORAL RESEARCH ASSOCIATE (advisor: Jorge Seminario)

**University of South Carolina, Columbia, SC**  
**Dept. of Chemical Engineering (January 1998-November 1999)**  
POSTDOCTORAL RESEARCH ASSOCIATE (advisor: Perla Balbuena)

**National University of Córdoba, Córdoba Argentina**  
**Dept. of Physics (August 1993-December 1997)**  
GRADUATE RESEARCH ASSISTANT  
TEACHING ASSISTANT  
**Dept. of Physics (August 1990-March 1991)**  
UNDERGRADUATE STUDENT ASSISTANT

### **SCIENTIFIC PUBLICATIONS**

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#### *i. Articles in Peer-Reviewed Journals*

23. "Molecular Rectifying Diodes Based on Aluminum /4'-Hydroxy-4-biphenyl Carboxylic Acid / p+-Silicon Junction" Bala, Sridevi; Aithal, Rajendra; Derosa, Pedro; Janes, David; Kuila, Debasish. Submitted to the Journal of Physical Chemistry, **2010**
22. "Poly(3-hexylthiophene) Nanotubes by Solution-Assisted Template Wetting" Joseph P. Cannon, Steven D. Bearden, LekhaNath Acharya, Pedro Derosa, and Scott A. Gold. Submitted to Synthetic Metals, **2010**
21. "Structural Patterns in (GaAs)<sub>n</sub> clusters", Gennady L. Gutsev, Mogus D. Mochena, Bidhan C. Saha, C. A. Weatherford and Pedro Derosa, Jr. Journal of Computational and Theoretical Nanoscience V. 7 (1) 254-263 **2010**
20. "A Combined Semiempirical-DFT Study of Large Oligomers within the Finite-Chain Approximation, Evolution from Oligomers to Polymers" Pedro A. Derosa Journal of Computational Chemistry, V. 30 (8), 1220-1228 **2009**
19. "Vibrational Study of a Molecular Device using Molecular Dynamics Simulations", Jorge M. Seminario, Pedro A. Derosa, Brian H. Bozard, and Krishna Chagarlamudi. Journal of Nanoscience and Nanotechnology, V. 5 (3), 484-495 **2005 Featured on the journal cover page**
18. "Nanometer-Size Conducting and Insulating Molecular Devices", Jorge M. Seminario, Cecilia E. De La Cruz, Pedro A. Derosa, and Liuming Yang. Journal of Physical Chemistry B, V. 108, 17879-17885 **2004**
17. "A Molecular Device Operating at Terahertz Frequencies", Jorge M. Seminario, Pedro A. Derosa, Luis Cordova, and Brian H. Bozard. IEEE transactions in Nanotechnology V. 3, 215-218, **2004**
16. "Molecular Electronics: Analysis and Design of Switchable and Programmable Devices Using Ab Initio Methods", Pedro A Derosa, Vandana Tarigopula, and Jorge M. Seminario. In Dekker Encyclopedia of Nanoscience and Nanotechnology. James A. Schwarz, Cristian Contescu, and Karol Putyera, editors. Marcel Dekker, Inc. New York. 2081-2099, **2004 Invited Paper**
15. "A programmable molecular diode driven by charge-induced conformational changes", Pedro A. Derosa, Suneel Guda, and Jorge M. Seminario. Communication to the Journal of the American Chemical Society V. 125, 14240-14241, **2003**

14. "An ab initio approach to the design flow of programmable molecular circuits", Jorge M. Seminario, Luis E. Córdoba, and Pedro A. Derosa. Proceedings of the IEEE V. 91. 1958-1975, **2003 Invited paper**
13. "Assessment of pulse height selection methods for several shapes in radiation detection", Raúl T. Mainardi, Tomás S. Plivelic, and Pedro A. Derosa, Nuclear Instruments, and Methods in Physics Research B. V. 201 (3) 525-534, **2003**
12. "Theoretical Interpretation of Switching in Experiments with Single Molecules", Jorge M. Seminario, Pedro A. Derosa, and Jimena L. Bastos. Communication to the Journal of the American Chemical Society V. 124, 10266-10267, **2002**
11. "Analysis of a Dinitro-based Molecular Device", Jorge M. Seminario, Angelica G. Zacarías, and Pedro A. Derosa. Journal of Chemical Physics V. 116, (4) 1671-1683, **2002**
10. "Molecular Gain in a Thiitolane System", Jorge M. Seminario and Pedro Derosa. Communication to the Journal of the American Chemical Society V. 123, 12418-12419, **2001**
9. "Properties of Small Bimetallic Ni-Cu Clusters", Pedro A. Derosa, Jorge M. Seminario, and Perla B. Balbuena. Journal of Physical Chemistry A V. 105, 7917-7925, **2001**
8. "A Theoretical Analysis of Metal-Molecule Contacts", Jorge M. Seminario, Cecilia E. De La Cruz, and Pedro A. Derosa. Communication to the Journal of the American Chemical Society V. 123, 5616-5617, **2001**
7. "Theoretical Analysis of Complementary Molecular Memory Devices", Jorge M. Seminario, Angelica G. Zacarías, and Pedro A. Derosa. Journal of Physical Chemistry A V 105 N° 5, 791-795, **2001 Featured on the journal cover page**
6. "Electron Transport through Single Molecules: Scattering Treatment using Density Functional and Green Function Theories", Pedro A. Derosa and Jorge M. Seminario. Journal of Physical Chemistry B V. 105 N° 2, 471-481, **2001**
5. "A Lattice-Gas Model Study of Lithium Intercalation in Graphite", Derosa P.A. and Balbuena P.B., Journal of the Electrochemical Society V 146 N° 10, 3630-3638, **1999**
4. "Density Functional Theory Study of Copper Clusters", Balbuena P.B., Derosa P.A. and Seminario J.M. Journal of Physical Chemistry B, V 103 N°15, 2830-2840, **1999**
3. "Absolute mass thickness determination of thin samples by X-ray fluorescence analysis", Barrea R., Bengió S., Derosa P and Mainardi R., Nuclear Instruments and Methods in Physics Research B. V 143 N° 4, 561-568, **1998**
2. "Parametric Equation for Efficiency Curve of Germanium Detectors", Víctor Delgado Martínez, Raúl T. Mainardi, Raúl A. Barrea, Carmen Martínez Hidalgo, Pedro A. Derosa and Marisa Marco Arbolí, X-Ray Spectrometry V 27, 321-324, **1998**
1. "Polarization of X-rays from the Interior of a Spherical Shell", Derosa P.A., Mainardi R.T., X-Ray Spectrometry, V. 25, 125-130, **1996**

## ***ii. Edited book***

Currently editing for CRC a book "Multiscale Modeling: From Atoms to Devices" Tahir Cagin co-editor

## ***iii. Peer reviewed Conference Proceedings***

5. "Search for Minimum Molecular Programmable Units", Jorge M. Seminario, Luis E. Córdoba, and Pedro A. Derosa. Second IEEE-nano Proceedings, V. 2, 421-424, **2002**

4. "Statistical Pulse Height Distribution Width Reduction by Suitable Selection of Amplitudes", Plivelic T., Derosa P., Bengió S. and Mainardi R., *Radiation Physics and Chemistry* V 51 N°4/6, 443-444, **1998**
3. "X-Ray Polarization Efficiencies of Flat and Cylindrical Surfaces", Derosa P. y Mainardi R., *Radiation Physics and Chemistry* V 51 N°4/6, 447, **1998**
2. "Thin Sample Thickness Determination by X-Ray Fluorescence Analysis", Barrea R., Derosa P., Bengió S. y Mainardi R., *Radiation Physics and Chemistry* V 51 N°4/6, 673, **1998**
1. "Calculations of X-Ray Beam Polarization in a Spherical Surface", Derosa P.A., Mainardi R.T., *Journal of Applied Radiation and Isotopes* V.46, N°6/7, 441-442, **1995**

#### *iv. Non-peer reviewed Conference Proceedings*

5. "Diffusion of Protons in Nanopores", Pedro Derosa, Bharat Kolan, and Scott Gold. *Proceedings of the AIChE Spring National Meeting*, April 22-27, **2007**.
4. "A Combined Model to Study Conductive Properties of Polymers with Atomic Resolution" Pedro Derosa, Kavitha Koraboina, Abdul Khaliq, and Mario Sanders. *Proceedings of the AIChE Fall National Meeting*, November 12-17, **2006**.
3. "First Principles Calculations on Cu and Cu-Ni Clusters", Derosa P., Balbuena P. and Seminario J. "Applying Molecular Modeling and Computational Chemistry" Topical Conference. *Proceedings of the AIChE annual meeting*, 315-322, **1998**
2. "Thin Film Thickness Determination by X-Ray Fluorescence", Barrea R.A., Mainardi R.T., Derosa P.A. y Bengió S., *Advances in Analysis by X-ray Techniques*. Vol. IX. *Proceedings - V SARX*, **1996**
1. "Calculations of X-ray Beam Polarization in a Spherical Surface", Derosa P.A., Mainardi R.T. *Advances in Analysis by X-ray Techniques*. Vol. VIII. *Proceedings - IV SARX*, **1994**

#### *v. Book Chapters*

3. "Molecular Dynamics Simulations of a Molecular Electronics Device: The NanoCell", Jorge Seminario, Pedro Derosa, Luis Cordova, and Brian Bozard, *Computational Chemistry*, review of current trends, World Scientific, V. 9, 85-119 **2005**
2. "Application of Density Functional Theory to the Study and Design of Molecular Electronic Devices: The Metal-Molecule Interface", Pedro A. Derosa, Angelica C. Zacarias, and Jorge M. Seminario. *Reviews in modern quantum chemistry: A celebration of the contributions of Robert G Parr*, Ed. Sen K.D., World Scientific, Singapore, 1537-1567, **2002**
1. "Ab Initio and Molecular Dynamics Studies of Cation-Water Interactions", Balbuena P.B., Wang L., Li T. and Derosa P.A., "Molecular Dynamics: from Classical to Quantum Methods", V. 7, "Theoretical and Computational Chemistry" Book Series, Ed. Balbuena P.B. and Seminario J.M., Elsevier Science Publishers, 431-469, **1999**

### **PRESENTATIONS IN SCIENTIFIC EVENTS**

#### *i. Invited talks*

14. "Electrical Conduction in Composites", Prairie View A&M University, Meeting of the Multiscale modeling team with Air Force POC, March 3, **2010**
13. "An Approach to Multi-Scale Modeling of Conductive Polymers" Southeastern Louisiana University, November 20, **2009**
12. "Electrical Conduction in Nanocomposites" Pedro Derosa 2009 Winter Review of the Minority Leaders Program, Air Force, Atlanta GA, February 18, **2009**

11. "Combined DFT/semiempirical approach, a tool for the multiscale modeling of conductive polymers" Pedro Derosa, Multiscale Modeling Invited Session, Boston, MA November 5<sup>th</sup>, **2008**
10. "The JFAP Summer Outreach Program". Pedro Derosa, Tabbetha Dobbins. 2008 Management Review meeting, Minority Leaders Program, Air Force. Dayton, OH, October 27<sup>th</sup>, **2008**
9. "Towards the Multi-scale Modeling of conductive polymers" Pedro A. Derosa, Annual Review and Workshop. Texas Institute for Intelligent Bio-Nano Materials and Structures for Aerospace Vehicles. August 8<sup>th</sup>, **2008**
8. "Multi-Scale Modeling of Conductive Polymers" Pedro Derosa. March Meeting of the APS, March 11, **2008**
7. "Modeling of the Electronic Behavior of CNT Composites". Pedro Derosa, 2008 Winter Review of the Minority Leaders Program, Air Force. New Orleans, LA, February 27<sup>th</sup>, **2008**
6. "The JFAP Summer Outreach Program". Pedro Derosa, Tabbetha Dobbins. 2008 Winter Review of the Minority Leaders Program, Air Force. New Orleans, LA, February 27<sup>th</sup>, **2008**
5. "Computer simulation, Vital Tool for Nanotechnology" Pedro Derosa. 50<sup>th</sup> Anniversary, Faculty of Mathematics, Astronomy, and Physics, Universidad de Córdoba, Argentina. December 21, **2006**
4. "Nanotechnology with Computers" Pedro Derosa. Universidad FASTA, Bariloche Argentina. August 8<sup>th</sup>, **2006**
3. "Molecular Simulation Study of Polymers", Pedro Derosa. School of Polymers and High Performance Materials of the University of Southern Mississippi, March 6<sup>th</sup>, **2006**
2. "Designing the Nanoworld with Computer Simulations", New Faculty Symposium Series, Louisiana Tech University, January 10<sup>th</sup>, and the Engineering and Science Board of Directors meeting, January 28<sup>th</sup>, **2006**
1. "Molecular Simulation, its Role in Nanotechnology", Derosa, P.A. Louisiana Academy of Science, Grambling, LA, March 18<sup>th</sup>, **2005**

## *ii. Contributions to Scientific meetings*

65. "Molecular Study of Charge Transport at the Interface between Nanostructures and Matrix in Nanocomposites" Pedro Derosa. March annual meeting of the American Physical Society, Portland, OR March 16, **2010**
64. "Polaron Transport in polymeric systems- A Monte-Carlo based Study" Deepti Shivane and Pedro Derosa The Louisiana Academy of Science Meeting, Alexandria, LA February 27, **2010**
63. "Polaron-Free Transport in Conductive Polymers using Monte-Carlo Simulations" Neha Ganapa and Pedro Derosa. The Louisiana Academy of Science Meeting, Alexandria, LA February 27, **2010 Selected finalist in the graduate student oral competition in the Physics, Chemistry and Earth Sciences division.**
62. "Molecular modeling scheme to efficiently determine the selectivity of various calix-crown molecules with Cs, K, and Na ions" Steven Baker, Bala Ramachandran, and Pedro Derosa The Louisiana Academy of Science Meeting, Alexandria, LA February 27, **2010 Winner for the graduate student oral competition in the Physics, Chemistry and Earth Sciences division.**
61. "A study of transport Phenomena in Nanostructures" Divya Elumalai, Vishwa Podduturi, and Pedro Derosa. The Louisiana Academy of Science Meeting, Alexandria, LA February 27, **2010**

60. "Study of geometrical structure and electronic properties of MEH-PPV" LekhaNath Acharya and P. Derosa, The Louisiana Academy of Science Meeting, Alexandria, LA February 27, **2010**
59. "Selective Complexation of Alkali Metal Cations with Calix[4]Crowns in Aqueous Media: A Density Functional Theory Study", Steven Baker, Bala Ramachandran, and Pedro Derosa The Louisiana Academy of Science Meeting, **Selected Finalist in the Graduate Student's Oral Competition**. Hammond, LA February 27, **2009**
58. "Linking Epon Polymers with Carbon Nanotubes", Stephen Ellis, Ross Beauttie, Steven Baker, and Pedro Derosa, The Louisiana Academy of Science Meeting, Hammond, LA February 27, **2009**
57. "Combined DFT/Semiempirical Approach, a Tool for the Multiscale Modeling of Conductive Polymers" Pedro Derosa. 236<sup>th</sup> fall National Meeting of the American Chemical Society, Philadelphia, Pennsylvania (August 17-21) **2008**
56. "Comparison of Four Different DFT Methods" Jasma Batham and Pedro Derosa. The Louisiana Academy of Science Meeting, **Selected Finalist in the Undergraduate Student's Oral Competition**, March 14, **2008**
55. "DFT Study of Molecular Toxicity", April Brandly and Pedro Derosa. The Louisiana Academy of Science Meeting, March 14, **2008**
54. "A Monte Carlo Approach to Electrical Conduction in Polymers", Nenian Charles and Pedro Derosa. The Louisiana Academy of Science Meeting, March 14, **2008**
53. "Molecular Diffusion using Monte Carlo Method", Leonid Kukuy, Pedro Derosa, and Michael Lewis. The Louisiana Academy of Science Meeting, March 14, **2008**
52. "Quantum mechanics study of electronic properties of polyanilines and Polypyrroles" Monica Bastola, Sudip Neupane, and Pedro Derosa. The Louisiana Academy of Science Meeting, March 14, **2008**
51. "Comparative Study of the Performance of DFT B3PW91 for the Prediction of Electronic Properties of Molecules" Jasma Batham and Pedro Derosa. March Meeting of the APS, March 12, **2008**
50. "Density Functional Theory Study of Polyanilines and Polypyrroles", Monica Bastola, Sudip Neupane, and Pedro Derosa. March Meeting of the APS, March 12, **2008**
49. "Monte Carlo Simulation Model for Charge Transport in Polymers" Nenian Charles and Pedro Derosa. TMS National Meeting, March 12, **2008**
48. "Diffusion of Species in Nanostructure". Pedro Derosa, Bharat Kolan, and Scott Gold. American Institute of Chemical Engineers (AIChE) Spring National, Houston, TX (April 22<sup>nd</sup>-27<sup>th</sup>) **2007**.
47. "Modeling Radiation Detectors Using Monte Carlo Simulations" Indraneel Sanikommu, Mahesh Neupane, and Pedro Derosa. Louisiana Academy of Science, 2007 meeting, Baton Rouge LA, March 16<sup>th</sup>, **2007. First place in the graduate student's poster competition**
46. "Proton Diffusion in Porous Materials, Molecular Dynamics Study" Bharat Kolan and Pedro Derosa. Louisiana Academy of Science, 2007 meeting, Baton Rouge LA, March 16<sup>th</sup>, **2007. Second place in the graduate student's poster competition**
45. "Efficient Monte Carlo Simulation algorithm for electron beam dosimetry in Electron beam Radiotherapy", Mahesh Neupane, Indraneel Sanikommu, and Pedro Derosa. Louisiana Academy of Science, 2007 meeting, Baton Rouge LA, March 16<sup>th</sup>, **2007**
44. "A Combined Model to Study Conductive Properties of Polymers with Atomic Resolution" Pedro Derosa, Kavitha Koraboina, and Brandon Howard. American Institute of Chemical Engineers (AIChE) Annual Meeting. San Francisco, CA (November 12<sup>th</sup>-17<sup>th</sup>) **2006**

43. "Using Computer-Interfaced Lab Sensors to Enhance Introductory Physics Laboratory", Pedro Derosa and Jenna Carpenter. 2006 AAPT Summer Meeting, Syracuse NY, July 22-26, **2006**
42. "Modeling Nanoparticle-Doped Radiation Detectors using Monte Carlo Simulations", Whitney C., Sanikommu I., Wilson C. and Derosa P.A. Louisiana Materials and Emerging Technologies Conference. Louisiana Tech University/ Grambling State University, Ruston LA, December 12-13, **2005**
41. "Proton Diffusion through Porous Materials, Molecular Simulation Approach" Kolan B. Gold S. and Derosa P.A. Louisiana Materials and Emerging Technologies Conference. Louisiana Tech University, Ruston LA, December 12-13, **2005**
40. "Molecular Dynamics Simulation of the Layer-by-Layer Assembly Process" Kolan B. and Derosa P.A. Louisiana Materials and Emerging Technologies Conference. Louisiana Tech University, Ruston LA, December 12-13, **2005**
39. "Detection of Cs<sup>+</sup> using Calix[4]arene-crown-6: Simulation-based Study" Suravhajula G., Varahramyan K., and Derosa P.A. Louisiana Materials and Emerging Technologies Conference. Louisiana Tech University, Ruston LA, December 12-13, **2005**
38. "Computational Study of Electronic, Geometrical, and Conductive Properties of Conductive Polymers", †Koraboina K., ‡Micheal T., and †‡Derosa P.A. Louisiana Materials and Emerging Technologies Conference. †Louisiana Tech University/ ‡Grambling State University, Ruston LA, December 12-13, **2005**
37. "Ab initio Study of the Selective Interaction of Calix[4]arene-Crown-6 with Alkali Metal Ions" Suravajhula, G. and Derosa, P.A. Louisiana Academy of Science, Grambling, LA, March 18<sup>th</sup>, **2005**
36. "Implementation of a Model for the Layer-by-Layer Assembly using Molecular Dynamics Simulations", Thippabathuni R. and Derosa, P.A. Louisiana Academy of Science, Grambling, LA, March 18<sup>th</sup>, **2005**
35. "Simulation Approach for the Design of Radiation Detectors", Derosa P.A., Chilla V.N., and Varahramyan K., AIChE Spring National meeting in Austin, TX in the session: Nanostructure Materials for Detection of Radioisotopes on November 11<sup>th</sup>, **2004**
34. "Nanostructure Materials for Detection of Radioisotopes", Derosa P.A., Sathyavada K., Suravhajula G.S., and Varahramyan K., AIChE Spring National meeting in Austin, TX in the session: Nanostructure Materials for Detection of Radioisotopes on November 11<sup>th</sup>, **2004**
33. "Computational Approach to Neutron Interactions: Combining Molecular Dynamics and Monte Carlo Simulations", Derosa P.A. The LONI Forum. Baton Rouge, Louisiana (September 2-3, **2004**)
32. "Computational Approach to Nanotechnology for Nuclear Non-Proliferation Applications", Derosa P.A. and Suravajhula G.S. Workshop on Nanotechnology for Nuclear Non-Proliferation Applications. Shreveport, Louisiana (July 26-27, **2004**)
31. "The Dinitropyridine Molecule: A Potential Molecular Switch", Derosa P.A., Guda S., and Seminario J.M. 225<sup>th</sup> Spring National Meeting of the American Chemical Society, New Orleans, Louisiana (March 23-27, **2003**)
30. "Study of the Role of Fluorinated Carbon Rings on the Chemical Physical and Conductive Properties of Phenyl-Based Oligomers", Derosa P.A., Bingi S., and Seminario J.M. SERMACS 2002 54<sup>th</sup> Regional Meeting of the American Chemical Society, Charleston, South Carolina (November 13-16, **2002**)
29. "Search for Minimum Molecular Programmable Units", Córdova L. A., Derosa, P. A., and Seminario J. M. US-Japan Moletronics Workshop, Chandler, Arizona (August 3<sup>rd</sup>, **2002**)

28. "Search for Minimum Molecular Programmable Units" First Mercury Poster, Conference in Computational Chemistry 2002, Pedro A. Derosa, Luis E. Cordova, Jorge M. Seminario, Clinton NY (July 21-23, **2002**)
27. "Electrical characterization of contact-molecule-contact", Figueroa H. P., Derosa P. A., Córdoba L. E. and Seminario J. M. Nanocenter Symposium, Columbia, South Carolina (April 19<sup>th</sup>, 2002)
26. "Analysis of Oxygen Density of States under Metallic Background", Araujo R. A., Agapito, L. A., Derosa P. A., Córdoba L. E. and Seminario J. M. Nanocenter Symposium, Columbia, South Carolina (April 19<sup>th</sup>, **2002**)
25. "Design and Analysis of a Dinitro-based Molecular Device", Derosa P. A., Zacarias A. G, and Seminario J. M. 41<sup>st</sup> Sanibel Meeting, St. Augustine, Florida. (February 24-March 2, **2001**)
24. "Theoretical Analysis of Metal-Molecule Interface", De La Cruz C. E., Derosa P. A., and Seminario J. M. 41<sup>st</sup> Sanibel Meeting, St. Augustine, Florida. (February 24-March 2, **2001**)
23. "Adsorption and Reaction on Copper, Nickel, and Copper-Nickel Systems", Derosa P.A., Mainardi D.S. and Balbuena P.B. American Institute of Chemical Engineers (AIChE) Annual Meeting. Dallas Texas. (October 30<sup>th</sup>-November 5<sup>th</sup>, **1999**)
22. "Calculations of Lithium Ion Intercalation in Graphitic Carbons", Derosa P.A., Marquez A.I. and Balbuena P.B. AIChE Annual Meeting. Dallas, Texas. (October 30<sup>th</sup>-November 5<sup>th</sup>, **1999**)
21. "Lattice Model Predictions of the Mechanisms of Ionic Intercalation in Graphite". American Physical Society (APS) Centennial Meeting. Atlanta, Georgia. (March 20<sup>th</sup>-26<sup>th</sup>, **1999**)
20. "First Principles Calculations of Cu and Cu-Ni Clusters", Derosa P.A., Balbuena P.B. and Seminario J.M., AIChE Annual Meeting. Miami, Florida. (November 15<sup>th</sup>-20<sup>th</sup>, **1998**)
19. "Study of the Mechanism of Intercalation of Lithium in graphite", Derosa P.A. and Balbuena P.B., AIChE Annual Meeting. Miami, Florida. (November 15<sup>th</sup>-20<sup>th</sup>, **1998**)
18. "First Principles-Based Calculation of Force-fields for Ion-Water Interactions", Balbuena P.B., Li T. Wang L. and Derosa P.A., AIChE Annual Meeting. Miami, Florida. (November 15<sup>th</sup>-20<sup>th</sup>, **1998**)
17. "Thickness Determination of Thin Films over substrate by XRFA", Barrea R., Bengiό S., Derosa P. and Mainardi R., 82nd. Argentine Physical Association (AFA) Meeting, San Luis-Argentina. (September 21<sup>th</sup>-26<sup>th</sup>, **1997**)
16. "Thin Film Thickness Determination by X-Ray Fluorescence Analysis", Barrea R., Derosa P., Bengiό S. and Mainardi R., 7<sup>th</sup> International Symposium on Radiation Physics. Jaipur-India (February 24<sup>th</sup>-28<sup>th</sup>) and School of Surface (EdeS). Buenos Aires-Argentina (July 14<sup>th</sup>-25<sup>th</sup>) **1997**
15. "X-Ray Polarization Efficiencies of Flat and Cylindrical Surfaces", Derosa P. and Mainardi R., 7<sup>th</sup> International Symposium on Radiation Physics. Jaipur-India. (February 24<sup>th</sup>-28<sup>th</sup>, **1997**)
14. "Statistical Pulse Height Distribution Width Reduction by Suitable Selection of Amplitudes", Plivelic T., Bengiό S., Derosa P. and Mainardi R., 7<sup>th</sup> International Symposium on Radiation Physics. Jaipur-India. (February 24<sup>th</sup>-28<sup>th</sup>, **1997**)
13. "Reduction of Relative Width of Statistical Distributions by Pulse Height Selection", Bengiό S., Plivelic T., Derosa P. and Mainardi R., 81st. AFA Meeting, Tandil-Argentina 1996. (September 16<sup>th</sup>-20<sup>th</sup>, **1996**)
12. "Thin-film Thickness Determination by X-ray Fluorescence", Barrea R., Mainardi R., Derosa P. and Bengiό S. V Symposium of X-Ray analysis (SARX), Cosquín-Argentina (November 19<sup>th</sup>-23<sup>th</sup>, **1996**)

11. "Comparison of Efficiency between a Plane X-ray Polarizer Device and a Cylindrical One ", Derosa P. and Mainardi R. 81st. AFA Meeting, Tandil-Argentina (September 16<sup>th</sup>-20<sup>th</sup>) and V SARX, Cosquín-Argentina (November 19<sup>th</sup>-23<sup>th</sup>) **1996**
10. "Germanium Detectors Efficiency Determination by Fitting a Monoparametric Model", Delgado Martínez V., Mainardi R.T., Barrea R.A., Martínez Hidalgo C., Derosa P.A. and Marco Arbolí M., European Conference on Energy Dispersive X-Ray Spectrometry. Lisbon-Portugal. (June 23<sup>th</sup>-29<sup>th</sup>, **1996**).
9. "Absolute Thickness Determination of Thin Film by X-ray Fluorescence", Mainardi R.T., Barrea R.A., Derosa P.A. y Bengió S., European Conference on Energy Dispersive X-Ray Spectrometry. Lisbon-Portugal. (June 23<sup>rd</sup>-29<sup>th</sup>, **1996**).
8. "X-ray Polarization by Dispersion in Curved Surfaces", Derosa P.A. y Mainardi R., VI Annual Workshop for Users, National Lab of Synchrotron Light (LNLS). Campinas-Brazil. (November 16<sup>th</sup>-17<sup>th</sup>, **1995**).
7. "XRF Determination of Concentrations and Thicknesses in Thin Samples", Bengió S., Derosa P., Barrea R. and Mainardi R., 80th. AFA Meeting, Bariloche-Argentina. (October 2<sup>nd</sup>-6<sup>th</sup>, **1995**).
6. "XRF through Reflection-transmission: Applications in Thin Films", Barrea R.A., Mainardi R.T., Bengió S. and Derosa P.A., Workshop on X-Ray Fluorescence with Synchrotron Radiation, Córdoba-Argentina. (September 6<sup>th</sup>-8<sup>th</sup>, **1995**).
5. "Design of an Experiment in Polarized Beam X-ray Fluorescence by Using the Monte Carlo Method", Derosa P.A., Mainardi R.T., Workshop on X-Ray Fluorescence with Synchrotron Radiation, Córdoba-Argentina. (September 6<sup>th</sup>-8<sup>th</sup>, **1995**).
4. "Calculations of X-ray Beam Polarization in a Spherical Surface", Derosa P.A., Mainardi R.T., 79th. Meeting of AFA, Córdoba (October 24<sup>th</sup>-29<sup>th</sup>) and IV SARX, Punta de Tralca-Chile. (October 24<sup>th</sup>-27<sup>th</sup>) **1994**
3. "Calculations of X-ray Beam Polarization in a Spherical Surface", Derosa P.A., Mainardi R.T., 6<sup>th</sup> International Symposium on Radiation Physics. Rabat-Morocco. (July 18<sup>th</sup>-22<sup>th</sup>, **1994**).
2. "Study of X-ray Polarization Characteristics by a B4C Cylinder", Derosa P.A., Mainardi R.T., 78th. AFA Meeting. Rosario-Argentina. (October 2<sup>nd</sup>-6<sup>th</sup>, **1993**).
1. "Study of Crystal Misorientation in Pure Ice Polycrystals". Derosa P.A., Neirotti J.P., Meriles C.A., Di Prinzio C.L., 75th. AFA Meeting. La Plata-Argentina. (October 8<sup>nd</sup>-11<sup>th</sup>, **1990**).

## **TEACHING EXPERIENCE**

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### **Louisiana Tech University, Physics program**

- *PHYS201*: Physics for Engineering and Science (Fall 2006 and Winter 2008-09)
- *PHYS533*: Statistical Mechanics (Co-taught, Winter 2007-08)
- *PHYS412/512*: Solid State Physics (Fall 2007 and Fall 2008)
- *CHEM586/450C*: Solid State Chemistry (Fall 2007)
- *PHYS522*: Quantum Mechanics (Spring 2006)
- *Integrated Science Curricula (ISC)*: Adapting labs on PHYS 261 and 262 to ISC (Fall 2004-current)
- *PHYS205*: Conceptual physics (Fall 2003, Winter and Spring 2004, Winter and Spring 2005, Winter 2007)
- *PHYS261*: General physics lab (Winter and Fall (2) 2004, Fall 2005)
- *PHYS262*: General physics lab (Fall 2003, Spring and Fall 2004, Winter, Spring, and Fall 2005, Winter 2006)

- *MSE504*: Advanced Material for Micro/Nano Devices and Systems. (Co-taught, Winter 2004) Lecturer
- 1-hour session for “Nanotechnology” (MSE 505) graduate course
- hour session for “Micro/Nano Scale Materials Measurements & Analysis” (MSE 506) graduate course

**Grambling State University, Department of Physics**

- *PHYS154*: General Physics II (Spring 2009)
- *PHYS154L*: General Physics II-Lab Section (Spring 2009)
- *PHYS152*: General Physics II (Spring 2006, 2007, and 2008)
- *PHYS152P*: General Physics II-Problem Session (Spring 2006, 2007, and 2008)
- *PHYS151L*: General Physics I-Lab Session (Fall 2007)
- *PHYS400*: Electronic Materials (Fall 2005)
- *SCI 103*: Physical Science Survey (Fall 1005)

**University of South Carolina, Dept of Chemistry and Biochemistry, Columbia, SC**

Lecturer

- Three 1-hour sessions for “Physical Chemistry” (Summer 2001) undergraduate course

**University of South Carolina, Dept of Chemical Engineering, Columbia, SC**

Lecturer

- 1-hour session for “Advanced Chemical Engineering Thermodynamics ” (fall 2001) graduate course
- 1-hour session for “Special Topics on Thermodynamics: Molecular Simulations” (Spring 1998) graduate course

National University of Córdoba, Córdoba Argentina.

***Teaching Assistant (March 1993-December 1997):***

Taught practical aspects of diverse undergraduate courses, including teaching lab, lecture presentation, exam preparation and grading.

- General Physics I, Dept. of Chemical Sciences (3 semesters).
- General Physics II, Dept. of Chemical Sciences (2 semesters).
- General Physics I, Dept. of Physics (2 semesters).
- Introduction to Physics, Dept. of Physics (2 semesters).
- Practical Course in PC operation, training course for University Staff, National University of Córdoba. (In charge of full course, dissertation, and practice)

***Undergraduate Teaching Assistant (February 1987-March 1993):***

Guided students in solving practical problems:

- Introductory course to University Studies, Dept. of Physics.
- Thermodynamics and Statistical Mechanics I, Dept of Physics

Modern Physics I, Dept of Physics.

**AWARDS AND SPECIAL ACCOMPLISHMENTS**

- **Co-Director**: Grambling State and Louisiana Tech University partners in the northern Louisiana Regional Collaborative
- **Chair**, Physics Section of the Louisiana Academy of Science, **August 2009-current**
- **Member of the editorial board**, Louisiana Academy of Science Proceedings, **August 2009-current**
- **Nominee Virgil Orr Undegraduate Junior Faculty Award**, voted to represent the College of Engineering and Science, Louisiana Tech University, **March 2009**

- **Task Leader**, multi-scale modeling team of the Air Force's Minority Leaders Program, **February 2009-current**
- **Subtask Leader**, atomic modeling within the multi-scale modeling team of the Air Force's Minority Leaders Program, **January 2008-February 2009**
- **Development of a Monte Carlo algorithm** to study hopping transport in conductive polymers. Disclosed to Louisiana Tech and Grambling State University, **2008**
- **Development of a Monte Carlo algorithm**, able to simulate interaction of radiation in nanoparticle containing systems. Disclosed to Louisiana Tech University, **2006**
- **Teacher's award**. Louisiana Tech University, September **2004**
- **Development** of a road map for the Department of Energy (DoE) on Nuclear Non-Proliferation applications. **Organizing committee member** of a workshop on nanotechnology for Nuclear Non-Proliferation applications where the roadmap was presented. The workshop was co-sponsored by DoE and held at the Institute for Micromanufacturing, Louisiana Tech University, June **2004**
- **ARO recognized** Prof. Jorge M. Seminario's molecular electronics group in ARO-in-review, for its achievements in 2002, particularly for the development of a combined Green function formalism and Density Functional theory technique I co-developed, **2003**
- **Presentation featured** in Chemical & Engineering News, "Computational nanotechnology", April 28 issue, page 27, **2003** Elizabeth K. Wilson editor
- **Software developed** together with Prof. Jorge Seminario implementing a combined Density Functional-Green function theory. Disclosed to the University of South Carolina, **2002**
- **Software developed** together with Prof. Perla Balbuena to study lithium intercalation on graphite based on a Lattice-gas model. License purchased by Mitsubishi Chemical Corporation (March **2001**)
- **IBM/Löwdin Fellowship Award** IBM/University of Florida at 41<sup>st</sup> Sanibel Symposium, St. Augustine, Florida (Feb 24-Mar 2, **2001**)
- **Principal Investigator** of 7 grants for Supercomputer time in different supercomputer facilities
- **Annual Award for Teacher** granted by the National University of Córdoba (**1994**)
- **Fellowship awarded** to carry out Ph.D. studies, Secretary of Science and Technology, National University of Córdoba (August 1993 -December 1997)
- **Fellowship awarded** to attend the "College on Computational Physics", International Center for Theoretical Physics, Trieste, Italy (May 15- June 9, 1995)

#### **OTHER ACTIVITIES**

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- Supervise four undergraduate student as part of the Rising Sophomore Academy, sponsored by the Center for Mathematical Achievement in Science and Technology (CMAST), Grambling State University, **May 2009**
- Supervise Two High School teacher on a 6 weeks research project as part of the Research Experience for Teachers. Louisiana Tech University, June 1-July 10, **2009**
- Supervise High School teacher on a 6 weeks research project as part of the Research Experience for Teachers. Louisiana Tech University, Summer, **2008** (1 teacher) and **2009** (two teachers)
- Deliver a workshop to high school teachers participating in a summer research experience for teachers (RET) on molecular simulations with application to alternative fuel sources. June **2008** and **2009**
- Representative of the Physics program in the integrated science curriculum (ISC) committee, Louisiana Tech University. Adapted two general physics labs to the ISC. **2004-2006**

- Judge Science Fair for the Red River Junior High School, (Represented GSU) February 1, **2006**
- Judge for Student oral and poster presentations on the 15<sup>th</sup> Annual Philip L. Young Research Symposium. Grambling State University, April 28, **2005**
- Scientific member of a South Carolina Department of Commerce mission to Seoul, Korea to assist to a demonstration of a new technology. Our evaluation was used to decide whether this technology should be brought to the State of South Carolina and to the University of South Carolina. **2001**
- Member of the Organizing Committee of V SARX held in Cosquín, Córdoba-Argentina, November 19 - 23, **1996**.
- Member of the board for Licenciado Carlos Pérez's thesis, "Experimental Methods and Techniques for the Determination of Depth Profiles by Total X-ray Reflection", March 23, **1995**.
- Secretary to the Cooperative Association, Faculty of Mathematics, Astronomy and Physics, from **June 19, 1994 to December 1997**.
- Selected as overseer Student at a Public Contest for Tenure (Faculty), November **1992**. Faculty of Mathematics, Physics, and Astronomy, National University of Córdoba.

## **FUNDING**

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### *i. Funded*

- 2010 JFAP Summer Outreach Research Program", Louisiana Board of Regents, \$60,381 (05/01/2009-04/30/2010) -**Current**
- "Conjugated Polymer Nanostructures for Supercapacitors and Batteries – Device Optimization and Modeling" Department of States (funded after an internal competition, College of Engineering and Science, Louisiana Tech University) (09/01/2009-08/31/2010)-**Current**
- "Multiscale Modeling of Thermal Transport in Electrically Active Nanocomposites", Air Force Research Lab, \$63,740 (09/01/2009-08/31/2010)-**Current**
- "Development of a Multi-scale Tool to Study Electronic, geometrical and Conductive Properties of Polymers", The Louisiana Board of Regents, \$129,871 (06/01/2009-05/31/2012) -**Current**
- 2009 JFAP Summer Outreach Research Program", Louisiana Board of Regents, \$20,000 (05/01/2009-04/30/2010) -**Current**
- "Minority leaders Materials and Manufacturing Research: Multiscale Modeling and Simulation of Materials Systems" (Member of the Modeling and Simulation Team), Air Force Research Lab, \$353,000 (09/01/2007-08/31/2010) -**Current**
- "A Realistic Model for Charge Transport in Conductive Polymers", The National Science Foundation and the Louisiana Board of Regents, \$10,000 (04/01/2008-03/31/2009)
- "Thermal Evaporator for Physics Education and Research", Louisiana Board of Regents, \$59,500 (04/01/2008-03/31/2009)
- "2007 JFAP Summer Outreach Research Program", Louisiana Board of Regents, \$22,500 (06/01/2007-09/30/2007)
- "2006 JFAP Summer Outreach Research Program", Louisiana Board of Regents, \$10,000 (06/01/2006-09/30/2006)
- "Nanoparticle-Based Scintillator for Enhanced Spatial Resolution and Selectivity for Neutron Detection-Phase II", Institute for Micromanufacturing, Louisiana Tech University (Funds for this internal program provided by DARPA), \$9,000 (07/16/2005-08/31/2006)

- “Study of Polymer Geometrical and Electronic Structure using Quantum Mechanics Calculations”, College of Engineering and Science, Louisiana Tech University, \$2,000 (06/01/2005-09/15/2005)
- “Nanoparticle-Based Scintillator for Enhanced Spatial Resolution and Selectivity for Neutron Detection-Phase I”, Institute for Micromanufacturing, Louisiana Tech University (Funds for this internal program provided by DARPA), \$10,000 (02/15/2005-07/15/2005)
- “2005 JFAP Summer Outreach Research Program”, Louisiana Board of Regents, \$10,000 (06/01/2005-09/30/2005)
- “IMR: Acquisition of a SGI Origin350 for Nano/Bio-Technology Computational Research and Student Training”, The National Science Foundation, \$119,649 (09/01/2004-08/31/2007)

### ***ii. Pending***

- “Enzyme encasing in clay tubes for nano-confined catalysis” The National Science Foundation, \$339,738 (03/01/2010-02/28/2013)
- “CAREER: A Multiscale Model for Charge Transport in Polymers and its Extension to Nanocomposites” The National Science Foundation, \$563,447 (03/01/2010-02/28/2015)

### **GRADUATE STUDENTS ADVISING**

#### •Graduate Student Research Advisors (committee Chair or co-Chair) for:

- Steven Baker (PhD, Computer Analysis and Modeling)
- Divya Elumalai (PhD, Engineering- Physics Track)
- David Cossey (PhD, Engineering -
- Deepti Shivane (PhD. Engineering – Microsystems Track)
- Karuna Yadla (MS. Electrical Engineering)
- Neha Ganapa (MS. Biomedical Engineering)

#### •Graduate Committee Member for:

- Joseph Canon (PhD-advisor Dr. Scott Gold)
- Brian Butcher (MSc-advisor Dr. Chad O’Neal)
- Hiu Wu (PhD-advisor Dr. Collin Wick)
- Xiang Li (PhD-advisor Dr. Frank Ji)
- Nagesh Idupulapati (PhD-Advisor Dr. Daniela Mainardi)
- Gopi Dathara (PhD-Advisor Dr. Daniela Mainardi)
- Veeramallu Rajeswari (PhD-Advisor Dr. Daniela Mainardi)
- Nagesh Idupulapati (MSc -Advisor Dr. Daniela Mainardi)
- Gopi Dathara (MSc. –grad 2006-Advisor Dr. Daniela Mainardi)

### **UNDERGRADUATE STUDENT MENTORING AND RESEARCH SUPERVISION**

- Sametra Delaney (GSU) Spring 2009-current
- Sparkle Springfield (GSU) Fall 2008-current
- Nenian Charles (GSU) Fall 2006-current
- Lekha Nath Acharya (LA Tech) Spring 2008-Current
- Tyler Michalak (LA Tech) January 2008-May 2009
- Travis J. King (LA Tech) Fall 2008-May 2009
- William Beattie (LA Tech) Summer 2008
- Stephen Travez Ellis (GSU) Summer 2008
- Leonid Kukuy (LA Tech) Spring 2007-Spring 2008
- Monica Bastola (LA Tech) Fall 2007-Spring 2008

- Sudip Neupane (LA Tech) Fall 2007-Spring 2008
- April Brandly (GSU-CMAST) Fall 2007-Spring 2008
- Leonid Kukuy (LA Tech) Spring 2007-Spring 2008
- Jasma Batham (LA Tech) Summer 2007
- Michael Lewis (LA Tech) Summer 2007
- Brandon Howard (GSU) Summer 2006- summer 2007
- Mario Sanders (GSU) Summer 2006
- Anthony Rugege (GSU) Summer 2005
- Antwan Lawrence (GSU) Summer 2005
- Tsega Michael (GSU) Summer 2005

### **PROFESSIONAL DEVELOPMENT**

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- QEM-CAREER workshop, New Orleans LA, February 27-28, 2009
- “Creating connections” Workshop. Program design to instruct faculty in creation connections with high school students and teachers. **2007-2008**
- “NERO” workshop series **2007-2008**
- “Workshop on Building Technologies”. Oak Ridge National Laboratory, Oak Ridge, TN, February 14-15, **2006**
- “Technical Assistant Workshop for the White House Initiative on Historically Black Colleges and Universities (HBCU)”, DoE. Clark Atlanta University, Atlanta, GA May 23, **2005**.
- “Active learning workshop” by Rich Felder and Rebecca Brent, Louisiana Tech University, September 4-5, 2003
- English Conversation I and II, and Advanced English Conversation I, II and III. Integral Institute of Languages, (1992-1996). Córdoba, Argentina
- Intensive English Program under the California Cultural English Program, International English Institute, Fresno, California - January 1995.
- Reading-Comprehension Course on Scientific-Technical Discourse, Language Laboratory, Dept. of Agricultural Sciences, National University of Córdoba, 1986.
- Completed Conversation I and II. Integral Institute of Languages, (1995-1996).

### **PARTICIPATION IN SCIENTIFIC ASSOCIATIONS**

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- Member of the American Physical Society (APS)
- Member of the American Chemical Society (ACS)
- Member of the Louisiana Academy of Science (LAS)
- Member of the American Association of Physics Teachers (AAPT)
- Member of the American Institute of Chemical Engineers (AIChE)

Dr. Pedro A. DEROSA  
September 1 , 2010