

PEDRO A. DEROSA

Ph.D. in Physics

Institute for Micromanufacturing/Physics Program
Louisiana Tech University
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Grambling State University
Grambling, LA 71245
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EDUCATION

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.

RESEARCH EXPERIENCE

Grambling State University-Louisiana Tech University

TENURE-TRACK 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. (Effective November 2004)

Louisiana Tech University, Ruston, LA

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

RESEARCH ASSOCIATE

- Characterize neutron radiation damage using Molecular Dynamics and Monte Carlo simulations
- Study production of secondary radiation using Monte Carlo simulations
- Study radioisotope interaction with nanoporous materials and nanoparticles using Density Functional Theory
- Model the Layer-by-Layer assembly using Density Functional Theory and Molecular Dynamics

University of South Carolina, Columbia, SC

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

Dept. of Chemistry and Biochemistry (*November 1999-August 2001*)

POSTDOCTORAL RESEARCH ASSOCIATE (advisor: Jorge Seminario)

* 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

Conducted computational research on electron transport through molecules and vibrational properties of small systems for molecular electronics:

- Developed a combined Density Functional Theory and Green function (DFT-GF) approach to study electron transport in molecules
- Characterized current-voltage characteristics of molecules using the DFT-GF approach
- Characterized metal-molecule interface using the DFT-GF approach
- Predicted current-voltages characteristics of molecular diodes, switches, amplifiers, conductors, and insulators. Some predictions were done before the corresponding experiments were performed.
- Studied vibrational modes and their potential use for signal processing using Molecular Dynamics. Terahertz molecular devices.

University of South Carolina, Columbia, SC

Dept. of Chemical Engineering (*January 1998-November 1999*)

POSTDOCTORAL RESEARCH ASSOCIATE (advisor: Perla Balbuena)

Conducted computational research in physical-chemistry including molecular structure characterization and reactions in bulk and at interfaces:

- Studied electronic structure and adsorption of small molecules on clusters using Density Functional Theory
- Studied lithium intercalation in graphite using own Lattice-gas-based theory implemented in a specially developed software
- Studied lithium intercalation in graphite using Molecular Dynamics

National University of Córdoba, Córdoba Argentina

Dept. of Physics (*August 1993-December 1997*)

GRADUATE RESEARCH ASSISTANT

Conducted atomic and nuclear spectrometry experimental and theoretical research on the study of x-ray interaction with matter:

- Designed a cylindrical x-ray polarizer
- Studied X-ray fluorescence produced by polarized and non-polarized x-ray beams
- Developed software to study x-ray interaction with matter and other related research

Dept. of Physics (*August 1990-March 1991*)

UNDERGRADUATE STUDENT ASSISTANT

- Conducted atmospheric physics research to study pure-ice crystal growth and measured grain border misorientations

SCIENTIFIC PUBLICATIONS

i. Articles in Peer-Reviewed Journals

22. "Structural Patterns in (GaAs)_n clusters, Gennady L. Gutsev, Mogus D. Mochena, Bidhan C. Saha, Pedro Derosa, and Charles W. Bauschlicher, Jr. Submitted to the Journal of Chemical Physics, **2009**
21. "Energy Band Gap in MEH-PPV and Energy Level Alignment at interface" David K. Chambers, Pedro A. Derosa, Orhan Kizilkaya, and Sandra Selmic. To be submitted to Polymer Engineering and Science. Summer **2009**
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, Published online November **2008**

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 (2), 1-11 **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 Thiotolane 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., Bengio 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

11. "Electrical Conduction in Nanocomposites" Pedro Derosa 2009 Winter Review of the Minority Leaders Program, Air Force, Atlanta GA, February 18, **2009**
10. "Combined DFT/semiempirical approach, a tool for the multiscale modeling of conductive polymers" Pedro Derosa, Multiscale Modeling Invited Session, Boston, MA November 5th, **2008**
9. "The JFAP Summer Outreach Program". Pedro Derosa, Tabbetha Dobbins. 2008 Management Review meeting, Minority Leaders Program, Air Force. Dayton, OH, October 27th, **2008**
8. "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 8th, **2008**
7. "Multi-Scale Modeling of Conductive Polymers" Pedro Derosa. March Meeting of the APS, March 11, **2008**
6. "Modeling of the Electronic Behavior of CNT Composites". Pedro Derosa, 2008 Winter Review of the Minority Leaders Program, Air Force. New Orleans, LA, February 27th, **2008**
5. "The JFAP Summer Outreach Program". Pedro Derosa, Tabbetha Dobbins. 2008 Winter Review of the Minority Leaders Program, Air Force. New Orleans, LA, February 27th, **2008**
4. "Computer simulation, Vital Tool for Nanotechnology" Pedro Derosa. 50th Anniversary, Faculty of Mathematics, Astronomy, and Physics, Universidad de Córdoba, Argentina. December 21, **2006**
3. "Nanotechnology with Computers" Pedro Derosa. Universidad FASTA, Bariloche Argentina. August 8th, **2006**
2. "Molecular Simulation Study of Polymers", Pedro Derosa. School of Polymers and High Performance Materials of the University of Southern Mississippi, March 6th, **2006**
1. "Designing the Nanoworld with Computer Simulations", New Faculty Symposium Series, Louisiana Tech University, January 10th, and the Engineering and Science Board of Directors meeting, January 28th, **2006**

ii. Contributions to Scientific meetings

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, Hammond, LA February 27, **2009**
58. "Linking Epon Polymers with Carbon Nanotubes", Stephen Ellis, Ross Beattie, 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. 236th 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 22nd-27th) **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 16th, **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 16th, **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 16th, **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 12th-17th) **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⁺ 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, 2005 meeting, Grambling, LA, March 18th, **2005**
36. "Molecular Simulation, its Role in Nanotechnology", Derosa, P.A. Louisiana Academy of Science, 2005 meeting, Grambling, LA, March 18th, **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 11th, **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 11th, **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. 225th 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 54th Regional Meeting of the American Chemical Society, Charleston, South Carolina (November 13-16, **2002**)
29. "Search for Minimum Molecular Programmable Units", Córdoba L. A., Derosa, P. A., and Seminario J. M. US-Japan Moletronics Workshop, Chandler, Arizona (August 3rd, **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 19th, 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 19th, **2002**)
25. "Design and Analysis of a Dinitro-based Molecular Device", Derosa P. A., Zacarias A. G, and Seminario J. M. 41st 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. 41st 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 30th-November 5th, **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 30th-November 5th, **1999**)
21. "Lattice Model Predictions of the Mechanisms of Ionic Intercalation in Graphite". American Physical Society (APS) Centennial Meeting. Atlanta, Georgia. (March 20th-26th, **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 15th-20th, **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 15th-20th, **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 15th-20th, **1998**)
17. "Thickness Determination of Thin Films over substrate by XRFA", Barrea R., Bengió S., Derosa P. and Mainardi R., 82nd. Argentine Physical Association (AFA) Meeting, San Luis-Argentina. (September 21th-26th, **1997**)
16. "Thin Film Thickness Determination by X-Ray Fluorescence Analysis", Barrea R., Derosa P., Bengió S. and Mainardi R., 7th International Symposium on Radiation Physics. Jaipur-India (February 24th-28th) and School of Surface (EdeS). Buenos Aires-Argentina (July 14th-25th) **1997**
15. "X-Ray Polarization Efficiencies of Flat and Cylindrical Surfaces", Derosa P. and Mainardi R., 7th International Symposium on Radiation Physics. Jaipur-India. (February 24th-28th, **1997**)
14. "Statistical Pulse Height Distribution Width Reduction by Suitable Selection of Amplitudes", Plivelic T., Bengió S., Derosa P. and Mainardi R., 7th International Symposium on Radiation Physics. Jaipur-India. (February 24th-28th, **1997**)
13. "Reduction of Relative Width of Statistical Distributions by Pulse Height Selection", Bengió S., Plivelic T., Derosa P. and Mainardi R., 81st. AFA Meeting, Tandil-Argentina 1996. (September 16th-20th, **1996**)
12. "Thin-film Thickness Determination by X-ray Fluorescence", Barrea R., Mainardi R., Derosa P. and Bengió S. V Symposium of X-Ray analysis (SARX), Cosquín-Argentina (November 19th-23th, **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 16th-20th) and V SARX, Cosquín-Argentina (November 19th-23th) **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 23th-29th, **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 23rd-29th, **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 16th-17th, **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 2nd-6th, **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 6th-8th, **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 6th-8th, **1995**).
4. "Calculations of X-ray Beam Polarization in a Spherical Surface", Derosa P.A., Mainardi R.T., 79th. Meeting of AFA, Córdoba (October 24th-29th) and IV SARX, Punta de Tralca-Chile. (October 24th-27th) **1994**
3. "Calculations of X-ray Beam Polarization in a Spherical Surface", Derosa P.A., Mainardi R.T., 6th International Symposium on Radiation Physics. Rabat-Morocco. (July 18th-22th, **1994**).
2. "Study of X-ray Polarization Characteristics by a B4C Cylinder", Derosa P.A., Mainardi R.T., 78th. AFA Meeting. Rosario-Argentina. (October 2nd-6th, **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 8nd-11th, **1990**).

TEACHING EXPERIENCE

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.

First Class Assistant (March 1993-March 2000):

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

- **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 41st 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

- Supervise one High School teacher on a 6 weeks research project as part of the Research Experience for Teachers. June 1-July 11, **2008**
- 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 23-24, **2008**
- Representative of the Physics program in the integrated science curriculum (ISC) committee. Adapted two general physics labs to the ISC. 2004-current
- Judge Science Fair for the Red River Junior High School, (Represented GSU) February 1, **2006**
- Judge for Student oral and poster presentations on the 15th 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

i. Funded

- “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)
- “Minority leaders Materials and Manufacturing Research: Multiscale Modeling and Simulation of Materials Systems” (Member of the Modeling and Simulation Team), Air Force Research Lab, \$214,000 (09/01/2007-08/31/2009)
- “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 II”, 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

- “High-end Scientific Visualization and Animation Enhancement to Computational Modeling Laboratory” The Louisiana Board of Regents, \$29,000 (07/01/2009-06/30/2010)
- “Development of a Multi-scale Tool to Study Electronic, geometrical and Conductive Properties of Polymers” The Louisiana Board of Regents, \$173,878 (07/01/2009-06/30/2012)
- “Development of Coarse-Graining Procedures for Multi-scale Modeling Studies” The National Science Foundation, \$399,745 (06/01/2009-05/31/2012)
- “Nanoprinted Enzyme Patterns in Microchannel Networks for Improved Practical Catalysis Applications” The National Science Foundation, \$558,897 (08/01/2009-07/31/2012)
- Combined Electrode-Mediator Nanostructures for Improved Electron Transport in Enzymatic Fuel Cell Anodes The National Science Foundation, \$595,758 (08/01/2009-07/31/2012)
- “Microscale Radiological, Environmental, and Biological Monitoring Microdevices for NASA Commercialization” NASA/The Louisiana Board of Regents, \$1,500,00 (08/01/2009-07/31/2012)

GRADUATE STUDENTS ADVISING

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

- Steven Baker (PhD, Computer Analysis and Modeling)
- Neha Ganapa (MS. Biomedical Engineering)
- Deepti Shivane (MS. Biomedical Engineering)
- Mahesh Neupane (PhD. Computer Analysis and Modeling)
- Chad Whitney (PhD. Engineering/Electrical)

•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 RESERCH SUPERVISION

- Sametra Delaney (GSU) Spring 2009-current
- Travis J. King (LA Tech) Fall 2008-current
- Sparkle Springfield (GSU) Fall 2008-current
- Nenian Charles (GSU) Fall 2006-current
- Tyler Michalak (LA Tech) January 2008-current
- Lekha Nath Acharya (LA Tech) Spring 2008-Current
- 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

- 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

- 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)

Dr. Pedro A. DEROSA
March 12th, 2009