Paulo H. Acioli

Physics and Astronomy Department
Northeastern Illinois University
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Degrees:

1995	Ph.D. In Physics. University of Illinois at Urbana Champaign
1991	M.Sc. in Physics University of Illinois at Urbana-Champaign
1988	Masters in Physics Universidade de Brasília, Brasília, Brazil

Professional Experience

Sep 2015 to Present	Professor Department of Physics and Astronomy, Northeastern Illinois University, Chicago, IL
Jan 2015 to June 2015	Visiting Professor Instituto de Fisica, Universidade de Brasília, Brasília, DF, Brazil
July 2011 to Present	Chair Earth Science, Environmental Science, and Physics, Northeastern Illinois University, Chicago, IL
Sep 2009 to Present	Associate Professor Department of Physics and Astronomy, Northeastern Illinois University, Chicago, IL
Sep 2006 to Aug 2009	Assistant Professor Department of Physics and Astronomy, Northeastern Illinois University, Chicago, IL
Sep 2005 to Aug 2006	Visiting Lecturer Physics and Astronomy Department, Northeastern Illinois University, Chicago, IL
Jan 2005 to Apr 2005 Jul 2004 to Sep 2004 Jan 2004 to Apr 2004 Jan 2001 to Jul 2003	Visiting Scholar Chemistry Division, Argonne National Laboratory, Argonne, IL
Aug 1996 to July 2005	Assistant Professor Instituto de Fisica, Universidade de Brasília, Brasília, DF, Brazil
Sep1995 to Jul 1996	Pos-Doctoral Researcher Instituto de Fisica, Universidade de Brasília, Brasília, DF, Brazil

Teaching Experience (Graduate)

Instituto de Física, Universidade de Brasilia, Brasilia, DF, Brazil

Topics of Molecular Physics 1 – Mar to Jul/96
Topics of Electronic Structure – Apr to Jul/99, and Aug to Dec/99
Elaboration of Ph.D. thesis project – Mar to Jul/2000
Group Theory Applications in Physics – Aug to Dec/2000
Quantum Theory 1 – Aug to Dec/2003
Topics of Electronic Structure – Sep to Dec/2004

Teaching Experience (Undergraduate)

Physics and Astronomy Department, Northeastern Illinois University, Chicago, IL

College Physics I	Spring 2006, Summer 2006, Fall 2006, Spring 2007, Spring 2008
College Physics II	Fall 2007, Fall 2008, Fall 2009, Spring 2010, Fall 2010, Spring 2011
Physics I Laboratory	Fall 2005, Spring 2006, Summer 2006, Spring 2007, Spring 2008. Spring 2017
Physics II Laboratory	Fall 2008, Fall 2009, Spring 2010, Fall 2010, Spring 16
Physics I with Calculus	Fall 2005, Spring 2006, Spring 2007
University Physics I with Lab	Fall 2013, Fall 2014, Fall 2015, Fall 2016
University Physics II	Spring 2009, Fall 2012
University Physics II with Lab	Spring 2013, Spring 2014, Spring 2016, Spring 2017
Physics II Seminar	Spring 2010, Fall 2010
Physics III	Spring 2009
Introductory Mathematical Physics	Fall 2005
Mechanics I	Fall 2008, Fall 2010
Quantum Mechanics I	Fall 2007, Fall 2009, Fall 2017
Modern Physics Lab	Spring 2011, Spring 2013
Thermal Physics	Spring 2012

Instituto de Física, Universidade de Brasilia, Brasilia, DF, Brazil

Physics 1 (Mechanics) –	Sep/96 to Feb/1997 and Mar to Aug/98
Experimental Physics 1 (Mechanics) –	Sep/96 to Feb/97, Apr to Jul/97, Aug to Dec/97, Mar to Aug/98, Oct/98 to Feb/99, Apr to Jul/99, Aug to Dec/2000 and Aug to Dec/2003.
Experimental Physics 2 –	Apr to Jun/2004, Sep to Dec/2004
Experimental Physics 2 to Chemists –	Sep/96 to Feb/97
Structure of Matter 2 (Atomic Physics) –	Apr to Jul/97
Structure of Matter 4 (Molecular Physics) –	Aug to Dec/97
Quantum Physics –	Oct/98 to Feb/99 and Apr to Jul/99
Quantum Mechanics –	Aug to Dec/99 and Mar to Jul/2000

Graduate Student Advising

1. Washington B. Silva, "Basis Functions for the Computation of Vibrational Spectra of Molecules using the Quantum Monte Carlo Method**."** M.Sc. dissertation, Instituto de Física, Universidade de Brasilia, Brasilia, DF, Brazil, 2000.

2. Washington B. Silva. "Vibrational Spectra of H_n^+ Clusters ." PhD Thesis, Instituto de Física, Universidade de Brasilia, Brasilia, DF, Brazil, (May 2004)

3. Angelo M. Maniero. "Study of Electronic Structure of Molecules: Application to the Generation of Potential Energy Surfaces and to the Electron-Molecule Elastic Scattering". Ph.D. Thesis, Instituto de Física, Universidade de Brasilia, Brasilia, DF, Brazil, (April 2003)

4. Nelson Fernando Cho. "Hydrogen bonding in Magnesium Clusters", M.Sc. dissertation, , Instituto de Física, Universidade de Brasilia, Brasilia, DF, Brazil, (July 2005).

Undergraduate Student Advising

1. Narin Ratanavade and Michael Cline (in collaboration with Dr. S. Srinivas) “Qualitative and Quantitative Analysis of Ag-Cluster/CO Interactions”, Fall 2007 and Spring 2008. NEIU
2. Michael Cline (in collaboration with Dr. S. Srinivas and Dr. A. Fraiman) "Quantum Chemical Analysis of the Diels-Alder Reaction using Gaussian 03". Fall 2006 and Spring 2007. NEIU
3. Serge Toguem, "Coanda and Bernoulli Effects", Fall 2006 and Spring 2007. NEIU.
4. Steve Burkland, “Computational Modeling of Cluster-molecule Systems”, Summer 2009 through Spring 2010.
5. Greg Freimark, “Computational Modeling of Cluster-molecule Systems”, Summer 2009 through Spring 2010.
6. Indira Bambur, “Computational Modeling of Cluster-molecule Systems”, Summer 2009 through Spring 2010.
7. Sean Jensen, “Molecular Dynamics/Monte Carlo Simulations of Physical Systems”, Summer 2010
8. Maksym Dzyz, “Molecular Dynamics/Monte Carlo Simulations of Physical Systems”, Summer 2010.
9. Jayati Gohel, “Molecular Dynamics/Monte Carlo Simulations of Physical Systems”, Summer 2010.
10. Matt Pembroke, “Molecular Dynamics/Monte Carlo Simulations of Physical Systems”, Summer 2010.
11. Steve Burkland, “Molecular Dynamics/Monte Carlo Simulations of Physical Systems”, Summer 2010.
12. Sergio Guerrero, “Designing and Implementing a Wind Generator at NEIU”, Summer 2012.
13. Max Hansen, “Designing and Implementing a Wind Generator at NEIU”, Summer 2012.
14. Thomas McLaughlin, “Designing and Implementing a Wind Generator at NEIU”, Summer 2012.
15. Esosa Ogbomo, “Designing and Implementing a Wind Generator at NEIU”, Summer 2012.
16. Steve Roothaan, “Designing and Implementing a Wind Generator at NEIU”, Summer 2012.
17. Caroline Williams, “Designing and Implementing a Wind Generator at NEIU”, Summer 2012.
18. Bryan Loeding, “Designing Laboratory and Computer Activities for Matter & Interactions”, Summer 2013.
19. Max Hansen, “Designing Laboratory and Computer Activities for Matter & Interactions”, Summer & Fall 2013, and Spring 2014.
20. Caroline Williams, “Self-Healing Quantum Monte Carlo Method for Excited State Vibrational Spectra of Floppy Molecules”, Fall 2013.
21. Bilguun S. Woods, “Self-Healing Quantum Monte Carlo Method for Excited State Vibrational Spectra of Floppy Molecules”, Fall 2013 and Spring 2014.
22. Cesar Bustos, “Molecular Dynamics Study of the Reaction of Carbon Monoxide with Small Silver Clusters”, Summer 2014.
23. David Capota, “Molecular Dynamics Study of the Reaction of Carbon Monoxide with Small Silver Clusters”, Summer 2014.
24. John Gonzales, “Molecular Dynamics Study of the Reaction of Carbon Monoxide with Small Silver Clusters”, Summer 2014.
25. Bilguun Woods, “Molecular Dynamics Study of the Reaction of Carbon Monoxide with Small Silver Clusters”, Summer 2014.
26. Cesar Bustos, “Dynamics studies of electronic and magnetic properties of graphene nanorribons”, Summer 2016.

Special Skills

Programming. Experienced with Windows, LINUX and UNIX operating systems, PC and Macintosh.

Publications

1. **P. H. Acioli**, J. Jellinek, Kit Bowen Jr, Photoelectron Spectra of Aluminum-Molybdenum Mixed Metal Clusters, manuscript in preparation to be submitted to Phys. Rev. B.
2. **P. H. Acioli** and G. Magela e Silva, Magnetic and Structural Properties of Mobius Graphene Sheets, manuscript in preaparation to be submitted to Phys. Rev. B.
3. **P. H. Acioli** and J. Jellinek, Theoretical Analysis of Photoelectron Spectra of Pure and Mixed Metal Clusters: Disentangling Size, Structure and Composition Effects, J. Chem. Phys. C **121,** 16665-16672 (2017).
4. Wiliam F. da Cunha, **Paulo H. Acioli**, Pedro Henrique de Oliveira Neto, Ricardo Gargano, and Geraldo Magela e Silva, "Polaron Properties in Armchair Graphene Nanoribbons", J. Phys. Chem. A **120(27),** 4893-4900 (2016).
5. Pedro Henrique de Oliveira Neto, Demério A. da Silva Filho, Luiz F. Roncaratti, **Paulo H. Acioli** and Geraldo Magela e Silva, "Low-Temperature Seebeck Coefficients for Polaron-Driven Thermoelectric Effect in Organic Polymers", J. Phys. Chem. A **120(27),** 4923-4927 (2016).
6. P. H. Oliveira Neto, Demétrio A. da Silva Filho, W. F. Cunha, **P. H. Acioli**, and G. M. E Silva, The Limit of Exciton Diffusion in Highly Ordered π-Conjugated Systems , J. Phys. Chem. C **119**,19654 (2015)
7. Bilguun S. Woods and **Paulo H. Acioli**, "Drag Assisted Simulated Annealing Method for Geometry Optimization of Molecules", Procedia Computer Science **51**,1878 (2015).
8. **Paulo H. Acioli** and Sudha Srinivas, "Silver and Gold Mediated Nucleobases Bonding", J. Mol. Mod. **20(8)**, 2391 (2014).
9. **Paulo H Acioli** and Sudha Srinivas, "Experiential Learning of Classical Mechanics Through Molecular Dynamics", Proceedings of the World Conference in Physics Education 2012, Istambul, Turkey (2014)
10. **Paulo H. Acioli**, Steve Burkland, and Sudha Srinivas, "An exploration of the potential energy surface of the seven atom silver cluster and a carbon monoxide ligand", Eur. Phys. J. D, 66 215 (2012).
11. A. M. Maniero, **P. H. Acioli**, G. M. e Silva , and, R. Gargano, "Theoretical calculations of a new potential energy surface for the H + Li_2 reaction", accepted for publication in Chem. Phys. Lett. (2010)
12. **P. H. Acioli**, N. Ratanavade, M. R. Cline, and S. Srinivas, Density functional Theory study of Ag-Cluster/CO Interactions, in ICCS 2009, Part II, Lecture Notes in Computer Science 5545, G. Allen et al., Eds., Springer-Verlag, Berlin-Heildelberg, 2009, pp. 203-210
13. **P. H. Acioli**, Z. Xie, B. J. Braams, and J. M. Bowman, Vibrational Ground State properties of H_5^+ and its Isotopomers from Diffusion Monte Carlo Calculations, J. Chem. Phys. **128**, 104318 (2008).
14. G. M. e Silva, R. Gargano, W. B. da Silva, L. F. Roncaratti, and **Paulo H. Acioli**, Quantum Monte Carlo and Genetic Algorithm Study of the Potential Energy Surface of the H5+ Molecule, Int. J. Quant. Chem. **108(13)**, 2318 (2008).
15. J. Jellinek and **P. H. Acioli**, Computational Electron Spectroscopy of Gas Phase Metal Clusters, in The Chemical Physics of Solid Surfaces, Vol. 12, Clusters: From Gas Phase to Deposited, D. Woodruff (Ed) (Amsterdan, Elsevier, 2007) p. 299-326.
16. J. Jellinek**, Paulo H. Acioli**, J. G.-Rodeja, W. Zheng, O. C. Thomas, and K. H. Bowen, Jr., Mn_n^- Clusters: Subnanometer Half-Metallicity, Phys. Rev. B. **74**, 153401 (2006)..
17. J. Jellinek and **P. H. Acioli**, Computational Electron Spectroscopy - Application to Magnesium Clusters, Lecture Series in Computer and Computational Sciences, Vol. 3. G. Marouis and T. Simos, Eds. VSP, Leiden, 2005, pp. 59 to 74.

18. J.-L. Wang, **P. H. Acioli**, and J. Jellinek, Structure and Magnetism of V_nBz_{n+1} Sandwich Clusters, J. Amer. Chem. Soc. (communications) **127** , 2812 (2005).
19. A. M. Maniero and **P. H. Acioli**, Potential energy curves of Li_2 and LiH from a full configuration interaction pseudopotential procedure. Int. J. Quant. Chem. **103**, 711 (2005).
20. Frederico V. Prudente, Luis S. Costa, and **Paulo H. Acioli**, Guiding Function and Basis Function Optimization in Correlation Function Quantum Monte Carlo Calculations of Vibrational Excited States in Molecules, J. Chem. Phys. A **108**, 1305 (2004).
21. J. Jellinek, and **P. H. Acioli**, Metal Clusters and Metallicity: The Paradigm of Magnesium, in "Metal Ligand Interactions Molecular-, Nano-, and Macro-Systems in Complex Environments", p. 121, Ed. by N. Russo, D. R. Salahub and M. Witko. (Kluwer Academic Publishers, 2003)
22. **P. H. Acioli** and J. Jellinek, Theoretical Determination of Electron Binding Energy Spectra of Anionic Magnesium Clusters. Eur. Phys. J. D **24**, 27 (2003).
23. J. Jellinek, and **P. H. Acioli**, Converting Kohn-Sham Eigenenergies into Electron Binding Energies. J. Chem. Phys. **118**, 7783 (2003).
24. J. Jellinek, and **P. H. Acioli**, "Magnesium Clusters: Structural and Electronic Properties and the Size-Induced Nonmetal-to-Metal Transition" Erratum, J. of Phys. Chem. A **107**, 1670 (2003)
25. W. B. Silva, E. A. Correa, **P. H. Acioli**, and R. Gargano, Quantum and Classical Study of the Vibrational States of H_2^+ and H_3^+ Molecules. Int. J. Quant. Chem. **95**, 149 (2003).
26. **P. H. Acioli** and J. Jellinek, Electron Binding Energies of Anionic Magnesium Clusters and the Nonmetal-to-Metal Transition. Phys. Rev. Lett. **89(21),** 213402 (2002)
27. J. Jellinek, and **P. H. Acioli**, Magnesium Clusters: Structural and Electronic Properties and the Size-Induced Nonmetal-to-Metal Transition. J. of Phys. Chem. A **106(45)**, 10919 (2002)
28. G. M. e Silva, and **P. H. Acioli**, Dynamical effects on the competition between polarons and bipolarons in conjugated polymers. Journal of Molecular Structure (THEOCHEM) **538**, 45 (2001)
29. C. S. Pinheiro, **P. H. Acioli** and G. M. e Silva, Logical switching with the use of bipolarons in conjugated polymers. Journal of Molecular Structure (THEOCHEM) **539**, 55 (2001)
30. W. B. Silva, and. **P. H. Acioli**, Trial wave functions for the calculation of vibrational states of molecules using quantum Monte Carlo. The Journal of Chemical Physics, **114(22)**, 9720 (2001).
31. F. V. Prudente, L. S. Costa, and **P. H. Acioli**, Correlation Function quantum Monte Carlo studies of rovibrational excited states in molecules. Journal of Physics B - Atomic Molecular and Optical Physics **33(22)**, R285 (2000)
32. L. S. Costa, F. V. Prudente, and **P. H. Acioli**, Generalized Rotating Wave Functions for Quantum Monte Carlo Calculations of Rovibrational levels of N-body Systems. Physical Review A., **61**, 12506 (2000)
33. **P. H. Acioli**, L. S. Costa, and F. V. Prudente, Quantum Monte Carlo study of vibrational states of Silanone. Chemical Physics Letters., **321**, 121 (2000)
34. L. S. Costa, F. V. Prudente, **P. H. Acioli**, J. J. S. Neto, and J. D. M. Vianna, A Study of Confined Quantum Systems using the Woods-Saxon Potential. Journal of Physics B - Atomic Molecular and Optical Physics. , **32**, 2461 (1999)
35. G. M. e Silva, and **P. H. Acioli**, Dynamics of Charge Propagation in Molecular Circuits, Journal of Molecular Structure(THEOCHEM) **464(1-3)**, 67 (1999)
36. G. M. e Silva, and **P. H. Acioli**, Investigation of Charge Transport in Molecular Switches with Neural Networks. Journal of Computational Chemistry. **20(10)**, 1060 (1999)
37. **P. H. Acioli** and J. J. S. Neto, Quantum Monte Carlo Calculation of the Vibrational Levels of Planar Acetylene. Journal of Molecular Structure(THEOCHEM) **464(1-3)** 145 (1999)

38. F. V. Prudente, and **P. H. Acioli**, Quantum Monte Carlo Study of rovibrational states of Molecular Systems. Chemical Physics Letters. **302/3(4)**, 249 (1999)
39. **P. H. Acioli**, L. S. Costa and F. V. Prudente, Quantum Monte Carlo Study of Rovibrational States Utilizing Rotating Wavefunctions: Application to H2O. J of Chem. Phys. **111**, 6311 (1999)
40. G. M. e Silva, **P. H. Acioli** and Y. Ono, Dynamics of Charge Propagation on Branching Off Conjugated Polymers. Journal of the Physical Society of Japan. , **67(11)**, 3881 (1998)
41. F. V. Prudente, **P. H. Acioli** and J. J. Soares Neto, The Fitting of Potential Energy Surfaces with Neural Networks: Application to the Study of Vibrational Levels of H3+. The Journal of Chemical Physics **109(20)**, 8801 (1998)
42. **P. H. Acioli** and G. M. e Silva, Dynamics of Charge Transfer in Molecular Switches, Synthetic Metals **87**, 249 (1997)
43. **P. H. Acioli**, G. M. e Silva, and A. C. Pedroza, Estimating the Correlation Energies of Diatomic Molecules and Atoms with Neural Networks, Journal of Computational Chemistry. **18**, 1407 (1997)
44. **P. H. Acioli**, Review of Quantum Monte Carlo and its Applications, Journal of Molecular Structure (THEOCHEM). , **394(2-3)**, 75 (1997)
45. **P. H. Acioli** and D. Ceperley, A Quantum Monte Carlo Study of Jellium Surfaces: Electronic Densities and Pair Correlation Functions. Physical Review B**, 54(24)**, 17199 (1996)
46. **P. H. Acioli** and D. Ceperley, The Generation of Pseudopotentials from Correlated Wave Functions. The Journal of Chemical Physics, **100(11)**, 8169 (1994)

Invited Talks

1. **P. H. Acioli**, Computational Photoelectron Spectroscopy of Mixed Metal Clusters, Energy, Materials, Nanotechnology Meeting on Quantum, Vienna, Austria, June 18-22, 2017

2. **P. H. Acioli**, Exciton Mobility in Organic Photovoltaic Materials, Energy, Materials, Nanotechnology Meeting, Beijing, China, April 21-25, 2016

3. **P. H. Acioli**, Computational Vibrational Spectroscopy using Correlation Function Quantum Monte Carlo, Cherry L. Emerson Center for Scientific Computation, Emory University, May 21, 2007.

4. **P. H. Acioli**, Computational Vibrational Spectroscopy, Department of Physics, NEIU, March 21, 2006.

5. **P. H. Acioli**, Metal Clusters and Metallicity, Department of Physics, NEIU, Nov. 15, 2005.

6. **P. H. Acioli**, Structural and Electronic Properties of Magnesium Clusters, III Meeting of the Brazilian Materials Research Society (SBPMAT), Foz do Iguaçu, Brazil, Oct. 10-13, 2004.

7. **P. H. Acioli,** Electronic and Vibrational Spectroscopy of Molecules and Clusters, II Workshop on Molecular Physics and Spectroscopy, Universidade Federal Fluminense, Niteroi, Brazil, Nov. 3 to Dec 3, 2004.

8. **P. H. Acioli,** Magnesium Clusters and the Size-Induced Non-Metal to Metal Transition. Workshop on the Simulation and Modeling of Nanostructures, International Centre for Condensed Matter Physics, Brasília, Brazil, Dec 2-5,2003.

9. **P. H. Acioli**, Transforming Kohn-Sham Eigenenergies into Electron Binding Energies: Theory and Applications to Atoms, Molecules, and Clusters. I Brazilian Meeting on Theoretical and Computational Physics, Brasília, DF, Brazil, April 6-9, 2003.

10. **P. H. Acioli**, The Quantum Monte Carlo Method, V Brazilian School of Electronic Structure, Águas de Lindóia, SP, Brazil, July 1996.

11. **P. H. Acioli**, Electronic Correlation and the Quantum Monte Carlo Method, VIII Brazilian Symposium of Theoretical Chemistry, Caxambu, MG, Brazil, November, 1995.

Papers in Congress

1. **P. H. Acioli** and S. Srinivas, " Silver and Gold mediated nucleobases bonding", Oral presentation at the 2013 Quitel (Theoretical Chemists of Latin Expression Conference), Granada, Spain, June 30-July 5, 2013.

2. **P. H. Acioli,** S. Burkland, and S. Srinivas, "An exploration of the potential energy surface of the seven atom silver cluster and a carbon monoxide ligand", Poster at the 2013 Quitel (Theoretical Chemists of Latin Expression Conference), Granada, Spain, June 30-July 5, 2013.

3. **Paulo H. Acioli**, Steve Burkland, and Sudha Srinivas, "An exploration of the potential energy surface of the seven atom silver cluster and a carbon monoxide ligand", Oral presentation at the Annual NEIU Faculty Research Symposium, Northeastern Illinois University, Chicago, IL, Nov. 16, 2012.

4. **Paulo H Acioli** and Sudha Srinivas, “Experiential Learning of Classical Mechanics Through Molecular Dynamics”, Oral presentation at the World Conference in Physics Education 2012, Istambul, Turkey, July 2012.

5. **Paulo Acioli**, M. Cline, N. Ratanavade, and Sudha Srinivas, “Density functional Theory study of Ag-Cluster/CO Interactions”, Oral Presentation at the International Conference in Computational Science 2009 (ICCS 2009), Baton Rouge, Louisiana, U.S.A., May 25-27, 2009

6. Narin Ratanavade, Michael Cline, Sudha Srinivas, and **Paulo Acioli**, "Density Functional Theory Analysis of Ag-Cluster/CO Interactions". Poster presented at the 40th Midwest Theoretical Chemistry Conference. University of Michigan, Ann Arbor, MI, June 26-28, 2008.

7. **Paulo H. Acioli**, Zhen Xie, Bastiaan J. Braams, Joel M. Bowman, "Vibrational Ground State Properties of H5+ and its Isotopomers from Diffusion Monte Carlo Calculations". Poster presented at the 40th Midwest Theoretical Chemistry Conference. University of Michican, Ann Arbor, MI, June 26-28, 2008.

8. **Paulo H. Acioli**, Zhen Xie, Bastiaan J. Braams, Joel M. Bowman, "Vibrational Ground State Properties of H5+ and its Isotopomers from Diffusion Monte Carlo Calculations". Poster presented at the Gordon Research Conference on Atomic and Molecular Interactions. Colby-Sawyer College, New London, NH, July 6-11, 2008.

9. **Paulo H. Acioli,** Study of Properties of Metallic Clusters using Density Functional Theory, Talk at the XXVIII National Meeting of Condensed Matter Physics, Santos, SP, Brazil, May 10-13, 2005.

10. Nelson F. Cho and **Paulo H. Acioli,** Study of Hydrogen Storage in Magnesium Clusters, Poster presented at the XXVIII National Meeting of Condensed Matter Physics, Santos, SP, Brazil, May 10-13, 2005.

11. Washington B.Silva and **Paulo H. Acioli***,* Quantum and Classical Study of the Vibrational States of the H_2^+, H_3^+, H_4^+, and H_5^+ Molecules, First International Meeting on Applied Physics (APHYS 2003), Badajoz, Spain, Oct. 13-18,2003.

12. Washington B.Silva and **Paulo H. Acioli**, Correlation Function Quantum Monte Carlo Study of the Vibrational Structure of H_n^+ Clusters, n=2-5, XII Brazilian Symposium of Theoretical Chemistry (XII SBQT), Caxambu, Brazil, Nov. 23-26,2003.

13. **P.H. Acioli** and J. Jellinek, Structures and Electron Binding Energy Spectra of Anionic Mixed Aluminum-Nickel Clusters, Talk at the 2003 Midwest Theoretical Chemistry Conference (MTWCC-2003), Ames, IA, June 12-14, 2003.

14. J. Wang, **P.H. Acioli** and J. Jellinek, Structural, Electronic, and Magnetic Properties of Vanadium Clusters and V-Benzene Complexes, Poster to be presented at the 2003 Midwest Theoretical Chemistry Conference (MTWCC-2003), Ames, IA, June 12-14, 2003.

15. A. M. Maniero, R. Gargano, and **P. H. Acioli**, Comparative study of the reaction H + Li_2 → LiH + Li, Poster Presented at the XXVI National Meeting of Condensed Matter Physics, Caxambu, MG, Brazil, May 6-10, 2003.

16. F. V. Prudente, L. S. Costa, and **P. H. Acioli**, Optimization of guiding basis functions for correlated Quantum Monte Carlo computation of Vibrational States of Molecules, Talk at the XXVI National Meeting of Condensed Matter Physics, Caxambu, MG, Brazil, May 6-10, 2003.

17. A. M. Maniero, R. Gargano, K. C. Mundim, **P. H. Acioli**, Construction of the Potential Energy Surface for the Reactive Process H + Li_2 → LiH + Li via Configuration Interaction and the Generalized Simulated Annealing, Poster Presented at the XXV National Meeting of Condensed Matter Physics, Caxambu, MG, Brazil, May, 2002.

18. **P.H. Acioli** and J. Jellinek, Structural Forms, Energies, And Electronic Properties of Neutral and Charged Magnesium Clusters, Talk at the APS March Meeting, Indianapolis, IN, March 2002.

19. J. Jellinek and **P.H. Acioli**, Electron Binding Energies of Anionic Magnesium Clusters and the Size-Induced Insulator-to-Metal Transition, Talk at the APS March Meeting, Indianapolis, IN, March 2002.

20. **P.H. Acioli** and J. Jellinek, Computing Electron Binding Energies Within Density Functional Theory, Poster presented at the 34 Midwest Theoretical Chemistry Conference, Minneapolis, MN, October 2001.

21. **P. H. Acioli** and J. Jellinek, Structural Forms, Energies and Electron Binding Energies of Anionic Magnesium Clusters, Poster presented at the 34 Midwest Theoretical Chemistry Conference, Minneapolis, MN, October 2001.

22. A. Maniero, and **P. H. Acioli**, Construction of Ab Initio Potential Energy Surface for Triatomic Molecules, Poster presented in the XI Brazilian Symposium of Theoretical Chemistry, November, 2001.

23. W. B. Silva, R. Gargano, and **P. H. Acioli**, Vibrational Spectra of H2+ and H2+, Poster presented in the XI Brazilian Symposium of Theoretical Chemistry, November, 2001.

24. A. M. Maniero, and **P. H. Acioli**, Construction of Potential Energy Surface of Diatomic Molecules using Pseudopotential, Poster Presented at the XXIII National Meeting of Condensed Matter Physics, São Lourenço, MG, Brazil, May, 2000.

25. W. B. Silva, and **P. H. Acioli**, Basis Functions for the Computation of Vibrational Spectrum of H2O utilizing the Quantum Monte Carlo Method, Poster Presented at the XXIV National Meeting of Condensed Matter Physics, São Lourenço, MG, Brazil, May, 2000.

26. **P. H. Acioli**, L. S. Costa and F. V. Prudente, Quantum Monte Carlo Determination of Ro-vibrational excited states of molecules, Talk at the XXIII National Meeting of Condensed Matter Physics, São Lourenço, MG, Brazil, May, 2000

27. **P. H. Acioli**, L. S. Costa and F. V. Prudente, Quantum Monte Carlo Method for the Determination of Ro-vibrational States of Molecular Systems, Poster presented at the Workshop on Photodynamics: From Isolated Molecules to Condensed Phases, Havana, Cuba, February 2000.

28. C. S. Pinheiro, **P. H. Acioli** and G. M. e Silva, Logical Switching using Bipolarons in Polypirrol, Poster presented at the X Brazilian Symposium of Theoretical Chemistry, Caxambu, MG, Brazil, November, 1999.

29. **P. H. Acioli** and A. M. Maniero, Construction of Potential Energy Surface of Diatomic Molecules using Pseudopotential, Poster presented at the X Brazilian Symposium of Theoretical Chemistry, Caxambu, MG, Brazil, November, 1999.

30. **P. H. Acioli**, L. S. Costa and F. V. Prudente Vibrational States of Silanone, Poster presented at the X Brazilian Symposium of Theoretical Chemistry, Caxambu, MG, Brazil, November, 1999.

31. W. B. Silva, and **P. H. Acioli**, Basis Functions for the Computation of Vibrational Spectrum of H3+ utilizing the Quantum Monte Carlo Method, Poster presented at the X Brazilian Symposium of Theoretical Chemistry, Caxambu, MG, Brazil, November, 1999.

32. G. M. e Silva, and **P. H. Acioli**, Dynamic Effects between Polarons and Bipolarons in Conjugated Polymers, Poster presented at the X Brazilian Symposium of Theoretical Chemistry, Caxambu, MG, Brazil, November, 1999.

33. L. S. Costa, F. V. Prudente, J. J. S, Neto and J. D. M. Vianna, A Study of Confined Quantum Systems using the Woods-Saxon Potential, Talk at the XXII National Meeting of Condensed Matter Physics, São Lourenço, MG, Brazil, May, 1999.

34. W. B. Silva, and **P. H. Acioli**, Basis Functions for the Computation of Vibrational Spectrum of Molecules, Poster Presented at the XXII National Meeting of Condensed Matter Physics, São Lourenço, MG, Brazil, May,1999.

35. **P. H. Acioli**, and G. M. e Silva, Investigation of the Charge Transport in Molecular Switches with Neural Networks , Poster Presented at the XXII National Meeting of Condensed Matter Physics, São Lourenço, MG, Brazil, 1999.

36. F. V. Prudente, and **P. H. Acioli**, Quantum Monte Carlo Study of Rovibrational States of Molecular Systems, Talk at the XXII National Meeting of Condensed Matter Physics, São Lourenço, MG, Brazil, 1999.

37. Paulo Hora Acioli, Geraldo Magela e Silva, Determination of a Molecular Logic Switch of Conducting Polymers using Neural Networks, Talk at the XXII National Meeting of Condensed Matter Physics, Caxambu, MG, Brazil, 1998.

38. Paulo Hora Acioli, J. J. S. Neto, 6-Dimensional Computation of the Vibrational Spectrum of Acetylene (HCCH),Talk at the XXII National Meeting of Condensed Matter Physics, Caxambu, MG, Brazil, 1998.

39. Frederico Vasconcellos Prudente, Paulo H. Acioli, J. J. Soares Neto, Computation of Potential Energy Surfaces Using Neural Networks, Talk at the XXII National Meeting of Condensed Matter Physics, Caxambu, MG, Brazil, 1998.

40. Frederico Vasconcellos Prudente, **Paulo H. Acioli**, J. J. Soares Neto, Computation of the Vibrational Spectrum of H3+ using Neural Networks and Quantum Monte Carlo, Talk at the XXII National Meeting of Condensed Matter Physics, Caxambu, MG, Brazil, 1998.

41. **P. H. Acioli**, Vibrational Spectra of Acetylene via Quantum Monte Carlo, Poster presented at the IX Brazilian Symposium of Theoretical Chemistry, Caxambu, MG, Brazil, November, 1997.

42. G. M. e Silva, and **P. H. Acioli**, Dynamic Study of Molecular Circuits of Polyacetylene, Poster presented at the IX Brazilian Symposium of Theoretical Chemistry, Caxambu, MG, Brazil, November, 1997.

43. **P. H. Acioli** and D. M. Ceperley, Exchange and Correlation Holes in Jellium Surfaces, Talk at the Electronic Exchange and Correlation in Advanced Materials Workshop (EXCAM-96), Ecole Politechnique, Palaiseau, Paris, France, September, 1996.

44. **P. H. Acioli** and D. M. Ceperley, Diffusion Monte Carlo Study of Metal Surfaces In The Jellium Model, Talk at the XX National Meeting of Condensed Matter Physics, Águas de Lindóia, SP, Brazil, 1996.

45. G. M. e Silva, **P. H. Acioli** and A. C. Pedroza, Estimating Correlation Energies Of Atoms And Diatomic Molecules With Neural Networks, Poster presented at the XX National Meeting of Condensed Matter Physics, Águas de Lindóia, SP, Brazil, 1996.

46. **P. H. Acioli** and D. M. Ceperley, A Quantum Monte Carlo Study of Jellium Surfaces: Electronic Densities and Pair Correlation Functions, Talk at the March Meeting of the American Physical Society, San Jose, CA, 1995.

47. **P. H. Acioli** and D. M. Ceperley, Variational Wave Function For Jellium Surfaces, Poster presented at the International Symposium on Electronic Structure, Santa Barbara, CA, 1994.

48. **P. H. Acioli** and D. M. Ceperley, Natural Orbitals of Lithium, Carbon and Neon using Quantum Monte Carlo, Talk at the March Meeting of the American Physical Society, Seattle, WA, 1993.

49. **P. H. Acioli** and N. S. Correa, A Study of Conductivity Parameters in Trans-Polyacetylene: Poster presented at the VI Latin American School of Theoretical Chemistry, Rio de Janeiro, RJ, Brazil, 1988.

Referee or Member of Editorial Board

Referee:

Physical Review A, B, E, Letters
Journal of Electron Spectroscopy and Related Phenomena
Chemical Physics Letters
New Journal of Physics
New Journal of Chemistry
Journal of Physical Chemistry
Journal of Molecular Structure(Theochem)
Journal of Molecular Modeling
Journal of Physics and Chemistry of Solids

Member of Editorial Board:

ISRN - Physical Chemistry Journal.
Journal of Modern Physics and Applications

Participation in Organizing Committees

XXII National Meeting of Condensed Matter Physics, São Lourenço, MG, Brazil, 1999.

VI Brazilian School of Electronic Structure, Santa Maria, RS, Brazil, July 1998.

Membership in Scientific Societies

American Physical Society (APS)

American Association of Physics Teachers (AAPT)

Funded Grants

PI (with other faculty in STEM) on the proposal "Peer Enhanced Experiential Research in STEM (PEERS)" submitted to the NSF-DUE-IUSE program. This project is designed to advance the research skills of undergraduate majors in STEM (Science, Technology, Engineering, and Mathematics) at Northeastern Illinois University (2014). $426,738.

CO-PI (with other faculty in STEM) on the NSF-S-STEM grant to create at Northeastern Illinois University (NEIU) a four-year support system for a cohort of motivated incoming freshmen in the STEM disciplines (2008)- $598,003

Awards

Argonne National Laboratory Pacesetter award for the extraordinary effort and efficiency in procurement, assembly, testing, and setting up a 128-processor Beowulf cluster. July 2002.

Finalist for 2016-2017 NEIU Bernard Brommel Distinguished Professor Award.