



Demétrio Antônio da Silva Filho

Curriculum Vitae

Personal Information

Name Demétrio Antônio da Silva Filho

Professional Address: Universidade de Brasília, Instituto de Física.

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Formal Education/Degree

- 1998 - 2003** Ph.D. in Physics
Universidade Estadual de Campinas, UNICAMP, Brasil with collaborative period at Universidade do Arizona (Advisor: Jean-Luc Brédas).
Year of degree: 2003.
Advisor: Maria Cristina dos Santos.
Scholarship from: Fundação de Amparo à Pesquisa do Estado de São Paulo , FAPESP , Brasil .
Keywords: Organic Semiconductors
Major Area: Exact and Earth Sciences / *Area:* Physics / *Subarea:* Atomic and Molecular Physics.
- 1996 - 1998** Master's in Physics
Universidade Federal de Pernambuco, UFPE, Brasil.
Year of degree: 1998.
Advisor: Celso Pinto de Melo.
Scholarship from: Coordenação de Aperfeiçoamento de Pessoal de Nível Superior, CAPES , Brasil .
Keywords: Polarizabilities; Organic Conducting Polymers.
Major Area: Exact and Earth Sciences / *Área:* Physics / *Subarea:* Atomic and Molecular Physics.
- 1992 - 1996** Graduation Physics
Universidade Federal de Pernambuco, UFPE, Brasil.
Advisor: Prof. Celso Pinto de Melo.
Scholarship from: Fundação de Amparo à Ciência e Tecnologia do Estado de Pernambuco , FACEPE , Brasil .

Postdoctorate

- 2003 - 2005** Postdoctorate.
Georgia Institute of Technology, Georgia Tech, Estados Unidos.
Scholarship from: National Science Foundation, NFS , Estados Unidos .
Major Area: Exact and Earth Sciences.
Major Area: Exact and Earth Sciences / *Área:* Physics / *Subarea:* Atomic and Molecular Physics.
- 2003 - 2003** Postdoctorate.
University of Arizona, ARIZONA, Estados Unidos.
Scholarship from: National Science Foundation, NSF , Estados Unidos .
Major Area: Exact and Earth Sciences.
Major Area: Exact and Earth Sciences / *Área:* Physics / *Subarea:* Atomic and Molecular Physics.

Professional Experience

University of Brasilia, UnB, Brazil.

2010 - Present Type of contract: Full-Professor, Exclusive Dedication.

Georgia Institute of Technology, GEORGIA TECH, United States.

2008 - 2009 Senior Research Scientist.

Articles in Scientific Journals

1. LEAL, LUCIANO ALMEIDA ; DE SOUSA, LEONARDO EVARISTO ; DE BRITO, PATRICK PASCOAL ; NETO, BERNHARD GEORG ENDERS ; CESCHIN, ARTEMIS MARTI ; DA CUNHA, WILIAM FERREIRA ; RIBEIRO, LUIZ ANTONIO ; SILVA FILHO, DEMÉTRIO ANTONIO DA . Optical properties of P3HT and N2200 polymers: a performance study of an optimally tuned DFT functional. JOURNAL OF MOLECULAR MODELING, v. 24, p. 32, 2018.
2. EVARISTO DE SOUSA, LEONARDO ; FERREIRA DA CUNHA, WILIAM ; ANTÔNIO DA SILVA FILHO, DEMÉTRIO ; DE OLIVEIRA NETO, PEDRO HENRIQUE . Biexciton cascade emission in multilayered organic nanofibers. APPLIED PHYSICS LETTERS, v. 112, p. 143301-143301, 2018.
3. EVARISTO DE SOUSA, LEONARDO ; DE OLIVEIRA NETO, PEDRO HENRIQUE ; Kjelstrup-Hansen, Jakob ; ANTÔNIO DA SILVA FILHO, DEMÉTRIO . Modeling temperature dependent singlet exciton dynamics in multilayered organic nanofibers. JOURNAL OF CHEMICAL PHYSICS, v. 148, p. 204101, 2018.
4. DE SOUSA, LEONARDO EVARISTO ; MAMIYA, ARTHUR AKIRA ; Kjelstrup-Hansen, Jakob ; DA SILVA FILHO, DEMÉTRIO ANTÔNIO . A joint theoretical and experimental characterization of two acene-thiophene derivatives. Journal of Molecular Modeling (Print), v. 23, p. 52-58, 2017.
5. KUKHTA, NADZEYA A. ; da Silva Filho, Demetrio A. ; VOLYNIUK, DMYTRO ; GRAZULEVICIUS, JUOZAS VIDAS ; SINI, GJERGJI . Can Fluorenone-based Compounds Emit in the Blue Region? Impact of the Conjugation Length and the Ground-State Aggregation. Chemistry of Materials, v. 29, p. 1695-1707, 2017.
6. PEREIRA, TAMIREZ LIMA ; LEAL, LUCIANO ALMEIDA ; DA CUNHA, WILIAM FERREIRA ; TIMÓTEO DE SOUSA JÚNIOR, RAFAEL ; RIBEIRO JUNIOR, LUIZ ANTONIO ; ANTONIO DA SILVA FILHO, DEMÉTRIO . Optimally tuned functionals improving the description of optical and electronic properties of the phthalocyanine molecule. Journal of Molecular Modeling (Print), v. 23, p. 71, 2017.
7. LEAL, LUCIANO ALMEIDA ; DA CUNHA, WILIAM FERREIRA ; RIBEIRO JUNIOR, LUIZ ANTONIO ; PEREIRA, TAMIREZ LIMA ; BLAWID, STEFAN MICHAEL ; DE SOUSA JUNIOR, RAFAEL TIMÓTEO ; DA SILVA FILHO, DEMÉTRIO ANTONIO . Optical and electronic structure description of metal-doped phthalocyanines. JOURNAL OF MOLECULAR MODELING, v. 23, p. 172, 2017.
8. LEAL, LUCIANO ALMEIDA ; DE SOUZA JÚNIOR, RAFAEL TIMÓTEO ; DE ALMEIDA FONSECA, ANTONIO LUCIANO ; RIBEIRO JUNIOR, LUIZ ANTONIO ; BLAWID, STEFAN ; DA SILVA FILHO, DEMETRIO ANTONIO ; DA CUNHA, WILIAM FERREIRA . Combined UMC- DFT prediction of electron-hole coupling in unit cells of pentacene crystals. JOURNAL OF MOLECULAR MODELING, v. 23, p. 153, 2017.
9. VOLPI, RICCARDO ; SANTOS CAMILO, ANA CLÁUDIA ; da Silva Filho, Demetrio A. ; NAVARRETE, J. TEODOMIRO LÓPEZ ; GOMEZ-LOR, BERTA ; RUIZ DELGADO, M. CARMEN ; LINARES, MATHIEU . Modelling Charge Transport of Discotic Liquid-Crystalline Triindoles: The Role of Peripheral Substitution. PHYSICAL CHEMISTRY CHEMICAL PHYSICS, v. 19, p. 24202-24208, 2017.
10. SOUSA, LEONARDO ; VOLPI, RICCARDO ; DA SILVA FILHO, DEMÉTRIO ANTÔNIO ; LINARES, MATHIEU . Mobility Field and Mobility Temperature Dependence in PC 61 BM: A Kinetic Monte-Carlo Study. CHEMICAL PHYSICS LETTERS, v. 689, p. 74-81, 2017.
11. LIMA, IGO T. ; SOUSA, LEONARDO ; FREITAS, RENATO DA S. ; JUNIOR, LUIZ ANTONIO RIBEIRO ; DE SOUSA JÚNIOR, RAFAEL TIMÓTEO ; da Silva Filho, Demétrio A. . A DFT study of a set of natural dyes for organic electronics. JOURNAL OF MOLECULAR MODELING, v. 23, p. 343, 2017.
12. DIAS LEDO, RODRIGO MAIA ; LEAL, LUCIANO ALMEIDA ; DE BRITO SILVA, PATRICK PASCOAL ; DA CUNHA, WILIAM FERREIRA ; DE SOUZA, LEONARDO EVARISTO ; ALMEIDA FONSECA, ANTONIO LUCIANO ; CESCHIN, ARTEMIS MARTI ; DA SILVA FILHO, DEMÉTRIO ANTONIO ; RIBEIRO JUNIOR, LUIZ ANTONIO . Modeling optical properties of polymer-solvent complexes: the chloroform influence on the P3HT and N2200 absorption spectra. JOURNAL OF MOLECULAR MODELING, v. 23, p. 1-8, 2017.1. CÂNDIDO, KAMILLA F. ; RAMALHO, SIMONE S. ; CUNHA, WILIAM F. DA ; SILVA FILHO, DEMÉTRIO A. DA . Strategies to Reduce the Computational Cost of the Ground State and the First Excited State Geometry Optimization of Organic Molecules. Revista Virtual de Química, v. 8, p. 356-368, 2016.
13. LIMA, IGO T. ; PRADO, ANDRIELE DA S. ; MARTINS, JOÃO B. L. ; DE OLIVEIRA NETO, PEDRO HENRIQUE ; CESCHIN, ARTEMIS M. ; da Cunha, Wiliam F. ; da Silva Filho, Demétrio A. . Improving the Description of the Optical Properties of Carotenoids by Tuning the Long-Range Corrected Functionals. The Journal of Physical Chemistry. A, v. 120, p. 4944-4950, 2016.
14. DE OLIVEIRA NETO, PEDRO HENRIQUE ; da Silva Filho, Demetrio A. ; RONCARATTI, Luiz Fernando ; ACIOLI, PAULO H ; E SILVA, GERALDO MAGELA . Low Temperature Seebeck Coefficients for Polaron Driven Thermoelectric Effect in Organic Polymers. The Journal of Physical Chemistry. A, v. 120, p. 4923-4927, 2016.
15. MOTA, ALBERTO A. R. ; CORRÊA, JOSÉ R. ; CARVALHO, PEDRO H. P. R. ; DE SOUSA, NÚBIA M. P. ; DE OLIVEIRA, HEIBBE C. B. ; GATTO, CLAUDIA C. ; da Silva Filho, Demétrio A. ; DE OLIVEIRA, ALINE L. ; NETO, BRENNO A. D. . Synthesis, Structure, Properties, and Bioimaging of a Fluorescent Nitrogen-Linked Bisbenzothiadiazole. Journal of Organic Chemistry, v. 81, p. 2958-2965, 2016.
16. DE SOUSA, LEONARDO EVARISTO ; RIBEIRO, LUIZ ANTONIO ; FONSECA, ANTONIO LUCIANO DE ALMEIDA ; DA SILVA FILHO, DEMÉTRIO ANTONIO . Modeling the Emission Spectra of Organic Molecules: A Competition between Franck-Condon and Nuclear Ensemble Methods. The Journal of Physical Chemistry. A, v. 120, p. 5380-5388, 2016.

17. MACHADO, DANIEL F. S. ; LOPES, THIAGO O. ; LIMA, IGO T. ; da Silva Filho, Demétrio A. ; DE OLIVEIRA, HEIBBE C. B. . Strong Solvent Effects on the Nonlinear Optical Properties of and Isomers from Azo-Enaminone Derivatives. *Journal of Physical Chemistry. C*, v. 120, p. acs.jpcc.6b01567-17669, 2016.
18. TAVARES, LUCIANA ; CADELANO, MICHELE ; QUOCHI, FRANCESCO ; SIMBRUNNER, CLEMENS ; SCHWABEGGER, GÜNTHER ; SABA, MICHELE ; MURA, ANDREA ; BONGIOVANNI, GIOVANNI ; FILHO, DEMÉTRIO ANTÔNIO DA SILVA ; DA CUNHA, WILIAM FERREIRA ; Rubahn, Horst-Günter ; Kjelstrup-Hansen, Jakob . Efficient Exciton Diffusion and Resonance-Energy Transfer in Multilayered Organic Epitaxial Nanofibers. *Journal of Physical Chemistry. C*, v. 119, p. 15689-15697, 2015.
19. DE OLIVEIRA NETO, PEDRO HENRIQUE ; da Silva Filho, Demétrio A. ; da Cunha, Wiliam F. ; ACIOLI, PAULO H. ; E SILVA, GERALDO MAGELA . Limit of Exciton Diffusion in Highly Ordered π -Conjugated Systems. *Journal of Physical Chemistry. C*, v. 119, p. 150819081507000-19659, 2015. Citações:1
20. RUIZ, CONSTANZA ; GARCÍA-FRUTOS, EVA M. ; da Silva Filho, Demetrio A. ; López Navarrete, Juan T. ; RUIZ DELGADO, M. CARMEN ; GÓMEZ-LOR, BERTA . Symmetry Lowering in Triindoles: Impact on the Electronic and Photophysical Properties. *Journal of Physical Chemistry. C*, v. 118, p. 5470-5477, 2014.
21. NETO, BRENNO A. D. ; H. G. DA CRUZ, EDUARDO ; H. P. R. CARVALHO, PEDRO ; CORRÊA, JOSÉ ; A. C. SILVA, DIEGO ; DIOGO, EMILAY ; SOUZA FILHO, JOSE D. ; CAVALCANTI, BRUNO ; PESSOA, CLÁUDIA ; GUIDO, BRUNA C. ; OLIVEIRA, HEIBBE C. B. ; SILVA FILHO, DEMETRIO A. ; SILVA JUNIOR, EUFRANIO . Design, synthesis and application of fluorescent 2,1,3-benzothiadiazole-triazole-linked biologically active lapachone derivatives. *New Journal of Chemistry (1987)*, v. NA, p. NA-NA, 2014.
22. DURÃES, JUSSARA A. ; da Silva Filho, Demétrio A. ; CESCHIN, ARTEMIS M. ; SALES, MARIA J. A. ; MARTINS, JOÃO B. L. . Investigation of the torsional barrier of EDOT using molecular mechanics and DFT methods. *Journal of Molecular Modeling (Print)*, v. 20, p. 2405-6, 2014.
23. Bredas, Jean-Luc ; LIMA, IGO T. ; RISKÓ, CHAD ; AZIZ, SAADULLAH ; DA SILVA FILHO, DEMETRIO . Interplay of Alternative Conjugated Pathways and Steric Interactions on the Electronic and Optical Properties of Donor-Acceptor Conjugated Polymers. *J MATER CHEM C*, v. 2, p. 8873-8879, 2014.
24. LOPES, THIAGO O. ; da Silva Filho, Demétrio A. ; LAPIS, ALEXANDRE A. M. ; DE OLIVEIRA, HEIBBE C. B. ; NETO, BRENNO A. D. . Designed non-symmetrical 4,7-pi-extended-2,1,3-benzothiadiazole derivatives: Synthesis guided by DFT predictions. *Journal of Physical Organic Chemistry (Print)*, v. 27, p. n/a-n/a, 2014.
25. FU, YAO-TSUNG ; da Silva Filho, Demetrio A. ; SINI, GJERGJI ; ASIRI, ABDULLAH M. ; AZIZ, SAADULLAH GARY ; RISKÓ, CHAD ; Brédas, Jean-Luc . Structure and Disorder in Squaraine-C 60 Organic Solar Cells: A Theoretical Description of Molecular Packing and Electronic Coupling at the Donor-Acceptor Interface. *Advanced Functional Materials (Print)*, v. 24, p. n/a-n/a, 2014.
26. da Silva Filho, Demetrio A. ; Coropceanu, Veaceslav ; Gruhn, Nadine E. ; DE OLIVEIRA NETO, PEDRO HENRIQUE ; Brédas, Jean-Luc . Intramolecular reorganization energy in zinc phthalocyanine and its fluorinated derivatives: a joint experimental and theoretical study. *Chemical Communications (London. 1996. Print)*, v. 49, p. 6069-6071, 2013.
27. DA SILVA FILHO, DEMETRIO A. ; DE OLIVEIRA NETO, PEDRO HENRIQUE ; RUIZ DELGADO, M. CARMEN ; LOPEZ NAVARRETE, JUAN T. ; Casado, Juan . Charge-transport in Organic Semiconductors: Probing High Mobility with Light. *MRS Proceedings*, v. 1568, p. mrs13-1568-kk12-05, 2013.
28. Casado, Juan ; Hernández, Víctor ; López Navarrete, Juan T. ; ALGARRA, MANUEL ; da Silva Filho, Demetrio A. ; YAMAGUCHI, SHIGEHIRO ; RONDÃO, RAQUEL ; SEIXAS DE MELO, J. SÉRGIO ; NAVARRO-FUSTER, VÍCTOR ; BOJ, PEDRO G. ; DÍAZ-GARCÍA, MARÍA A. . Amplified Spontaneous Emission in Pentathienoacene Dioxides by Direct Optical Pump and by Energy Transfer: Correlation with Photophysical Parameters. *Advanced Optical Materials*, v. 1, p. n/a-n/a, 2013.
29. RONCARATTI, Luiz Fernando ; GARGANO, R. ; OLIVEIRA NETO, P. H. ; CUNHA, Wiliam F da ; Filho DADS ; SILVA, Geraldo Magela e . Temperature-induced oscillating electric dipole in conjugated systems. *Chemical Physics Letters (Print)*, v. 539, p. 214-217, 2012.
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32. Delgado, M. Carmen Ruiz ; Kim, Eung-Gun ; Filho, Demetrio A. da Silva ; Bredas, Jean-Luc . Tuning the Charge-Transport Parameters of Perylene Diimide Single Crystals via End and/or Core Functionalization: A Density Functional Theory Investigation. *Journal of the American Chemical Society (Print)*, v. 132, p. 3375-3387, 2010.
33. Oliva, María Moreno ; Pappenfus, Ted M. ; Melby, Jacob H. ; Schwaderer, Kathryn M. ; Johnson, Jared C. ; McGee, Kari A. ; da Silva Filho, Demetrio A. ; Bredas, Jean-Luc ; Casado, Juan ; López Navarrete, Juan T. . Comparison of Thiophene-Pyrrole Oligomers with Oligothiophenes: A Joint Experimental and Theoretical Investigation of Their Structural and Spectroscopic Properties. *Chemistry - A European Journal*, p. n/a-n/a, 2010.

34. Pappenfus, Ted M. ; Hermanson, David L. ; Kohl, Stuart G. ; Melby, Jacob H. ; Thoma, Laura M. ; Carpenter, Nancy E. ; da Silva Filho, Demetrio A. ; Bredas, Jean-Luc . Regiochemistry of Poly(3-hexylthiophene): Synthesis and Investigation of a Conducting Polymer. *Journal of Chemical Education*, v. 87, p. 522-525, 2010.
35. Delgado, M. Carmen Ruiz ; Pigg, Kathryn R. ; da Silva Filho, D. A. ; Gruhn, Nadine E. ; Sakamoto, Youichi ; Suzuki, Toshiyasu ; Osuna, Reyes Malave ; Casado, Juan ; Hernández, Víctor ; Navarrete, Juan Teodomiro Lopez ; Martinelli, Nicolas G. ; Cornil, Jérôme ; Sánchez-Carrera, Roel S. ; Coropceanu, Veaceslav ; Brédas, J. L. . Impact of Perfluorination on the Charge-Transport Parameters of Oligoacene Crystals. *Journal of the American Chemical Society (Print)*, v. 131, p. 1502-1512, 2009.
36. Martinelli, Nicolas G. ; Olivier, Yoann ; Athanasopoulos, Stavros ; Ruiz Delgado, Mari-Carmen ; Pigg, Kathryn R. ; da Silva Filho, D. A. ; Sánchez-Carrera, Roel S. ; Venuti, Elisabetta ; Della Valle, Raffaele G. ; Brédas, Jean-Luc ; Beljonne, David ; Cornil, Jérôme . Influence of Intermolecular Vibrations on the Electronic Coupling in Organic Semiconductors: The Case of Anthracene and Perfluoropentacene. *ChemPhysChem*, p. NA-NA, 2009.
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Academic Advisory

Academic Advisory - current

Master's Thesis

1. Carlos Alberto Moreira de Melo Neto. Begin: 2014. Dissertation (Master's in Física) - Universidade de Brasília. (Advisor).
2. Antonio Marcos Silva Santos. Begin: 2014. Dissertation (Master's in Física) - Universidade de Brasília, Coordenação de Aperfeiçoamento de Pessoal de Nível Superior. (Advisor).

Ph.D. Thesis

1. Ana Cláudia Santos Camilo. Begin: 2015. Tese (Ph.D. in Física) - Universidade de Brasília, Coordenação de Aperfeiçoamento de Pessoal de Nível Superior. (Advisor).
2. Tamires Lima Pereira. Begin: 2015. Tese (Ph.D. in Física) - Universidade de Brasília, Coordenação de Aperfeiçoamento de Pessoal de Nível Superior. (Advisor).
3. Leonardo Evaristo de Sousa. Begin: 2015. Tese (Ph.D. in Física) - Universidade de Brasília, Coordenação de Aperfeiçoamento de Pessoal de Nível Superior. (Advisor).
4. Arthur Akira Mamiya. Begin: 2015. Tese (Ph.D. in Física) - Universidade de Brasília, Coordenação de Aperfeiçoamento de Pessoal de Nível Superior. (Advisor).

Scientific Initiation

1. Lethicia Vieira Marques. Begin: 2013 - Universidade de Brasília. (Advisor).

Academic Advisory - concluded

Master's Thesis

1. Tamires Lima Pereira. 2012. Dissertation (Master's in Physic) - Universidade de Brasília, Conselho Nacional de Desenvolvimento Científico e Tecnológico. *Advisor:* Demétrio Antônio da Silva Filho.
2. Ana Cláudia Santos Camilo. 2012. Dissertation (Master's in Physic) - Universidade de Brasília, Coordenação de Aperfeiçoamento de Pessoal de Nível Superior. *Advisor:* Demétrio Antônio da Silva Filho.

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1. Igo Torres Lima. 2010. Thesis (Ph.D. in Physic) - Universidade de Brasília, Coordenação de Aperfeiçoamento de Pessoal de Nível Superior. *Advisor:* Demétrio Antônio da Silva Filho.

Scientific Initiation

1. Guilherme Lucas Maciel Fernandes. 2012. Scientific Initiation - Universidade de Brasília, Conselho Nacional de Desenvolvimento Científico e Tecnológico. *Advisor:* Demétrio Antônio da Silva Filho.
2. Guilherme Ferreira. 2012. Scientific Initiation - Universidade de Brasília, Conselho Nacional de Desenvolvimento Científico e Tecnológico. *Advisor:* Demétrio Antônio da Silva Filho.
3. Walter Rodrigo Araújo Gregoldo. 2012. Scientific Initiation - Universidade de Brasília. *Advisor:* Demétrio Antônio da Silva Filho.
4. Sergio Fernandes da Silva Reis. 2012. Scientific Initiation - Universidade de Brasília, Conselho Nacional de Desenvolvimento Científico e Tecnológico. *Advisor:* Demétrio Antônio da Silva Filho.
5. Gabriel Fávero. 2010. Scientific Initiation - Universidade de Brasília. *Advisor:* Demétrio Antônio da Silva Filho.