

Antonio José Roque da Silva

Biographical information

Professor Antônio José Roque da Silva completed his bachelor's degree (1983-1986) and master's degree (1986-1989) in Physics at the Gleb Wataghin Institute of Physics (IFGW) at UNICAMP, Brazil. During his master's degree, he has worked on theoretical studies of spatial pattern formation and electron scattering by molecules. Between 1989 and 1994, he pursued his PhD at the Department of Physics, University of California at Berkeley under the supervision of Prof. Leopoldo Falicov. The title of his thesis was Magnetic and Optical Properties of Transition-Metal Halides and Solid Oxygen, and one of the notable results was the explanation of the contribution of magnetic entropy to the transition between the antiferromagnetic phase α -oxygen and the phase β -oxygen. Subsequently, he has worked at the Department of Chemistry and Biochemistry at the University of California, Los Angeles (UCLA), USA, in Prof. Emily Carter's group, focusing on quantum chemistry. His work focused on computational simulation using ab initio molecular dynamics methods. Notably, he studied the desorption of H_2 molecules from the (100) surface of Si, which was one of the first works using first-principles molecular dynamics to study reaction dynamics on surfaces. He also participated in the first work that aimed to integrate quantum chemistry and Density Functional Theory methods to treat correlated regions of an extended system via embedding techniques. In 1997, he joined the Institute of Physics at the University of São Paulo (USP), Brazil, as an assistant professor, initiating several projects in electronic structure calculations and computational simulations in various materials, with particular emphasis on nanostructures. It is worth mentioning his work on metallic nanowires, as well as on many other problems, such as carbon nanotubes, oxides, defects in semiconductors, surfaces, semiconductor nanowires, molecular electronics, and 2D materials, all with results regularly published in high-impact journals and conducted in collaboration with a variety of research groups in Brazil. He has also worked on the charge transport problem in nanostructures, participating in the development of the first Brazilian code for an ab initio calculation of these properties, TRANSAMPA. An important work in this area is the development of a method to treat via ab initio techniques the problem of charge transport in large and disordered systems (tens of thousands of atoms), allowing a realistic treatment of nano-sensors (Phys. Rev. Lett. 100, 176803 (2008)). He became associate professor (Livre Docente) in 2003, and Full Professor in 2008. He has published more than 130 articles in international journals, has participated in over 100 examination boards and committees (evaluations, competitions, doctoral and master's degrees), delivered more than 200 invited talks at conferences, workshops, and universities (both national and international), and has served on several organizing committees for national and international conferences, advisory committees, and the Brazilian Physics Olympiad. He has presented more than 230 papers at national and international conferences and is a level 1A Conselho Nacional de Desenvolvimento Científico e Tecnológico (CNPq) researcher. He has

supervised 22 master's, doctoral, and postdoctoral students. From 2008 to 2018, he served as one of the Physics Area coordinators at FAPESP, as a member of the Technical Scientific Council (CTC) of many scientific institutions in Brazil (LNA, INPE, and CBPF), and as a Member of the International Scientific Committee of the Kurchatov Institute (Russia). He has participated in Search Committees for Director's positions of many institutions, such as CBPF (twice, once as chair), INPE, CTI (as chair), and ON, and was a member of the Advisory Scientific Committee of the Brazilian Nanotechnology Program (MCTIC, 2011-2017). Since 2021, he has been a Member of the Superior Council of the National Association of Research and Development of Innovative Companies (ANPEI). He has received the 100 MOST INFLUENTIAL IN ENERGY award in 2018 and 2019, in the Research, Innovation, and Technology category, by Grupo Mídia, and the 100 MOST INFLUENTIAL IN ENERGY OF THE DECADE award, 2020, by Grupo Mídia as well. He is a full member of the Brazilian Academy of Sciences (ABC) and the São Paulo State Academy of Sciences (ACIESP) and was honored in 2018 with the National Order of Scientific Merit - Comendador Class. From 2009 until 2018, he has worked as Director of the Brazilian Synchrotron Light Laboratory (LNLS), one of the units of the Brazilian Center for Research in Energy and Materials-CNPEM. In 2018 Prof. Antônio José Roque da Silva became Director General of CNPEM. During this period, he has led the project for the construction of the new Brazilian 4th generation synchrotron light source, Sirius. This is the largest scientific equipment ever built in Brazil, a state-of-the-art synchrotron, designed to have the highest brightness in its energy class. Besides Sirius, he has also been leading the project and construction of another important and unique project in Brazil and Latin America, the so-called Orion. This will be a complex of high and maximum containment laboratories to study a variety of pathogens, including those classified and BSL-4. It will be the first of this category in Latin America, and the very first in the world connect to a synchrotron source, Sirius. Besides Sirius and Orion, Prof. Roque da Silva coordinates, together with all the Directors of the units of CNPEM, a variety of activities in the fields of nanotechnology, biosciences, biorenewables, and scientific instrumentation and engineering.

Articles

1. Fonseca, M. D.; Araujo, B. H. S.; Dias, C. S. B.; Archilha, N. L.; Neto, D. P. A.; Cavalheiro, E.; Westfahl, H.; da Silva, A. J. R.; Franchini, K. G.
High-resolution synchrotron-based X-ray microtomography as a tool to unveil the three-dimensional neuronal architecture of the brain
Scientific Reports, V. 8, P. 12074, 2018
2. Pontes, R. B.; Miwa, R. H.; da Silva, A. J. R.; Fazzio, A.; Padilha, J. E.
Layer-Dependent Band Alignment of Few Layers of Blue Phosphorus and their Van Der Waals Heterostructures With Graphene.
Physical Review B, V. 97, P. 235419, 2018.
3. Acosta, C. M.; Lima, M. P.; da Silva, A. J. R.; Fazzio, A.; Lewenkopf, C. H.

Tight-Binding Model for the Band Dispersion in Rhombohedral Topological insulators Over the Whole Brillouin Zone.
Physical Review B, V. 98, P. 035106, 2018.

4. Lima, M. P.; Fazzio, A.; da Silva, A. J. R.
Silicene-Based Fet for Logical Technology.
IEEE Electron Device Letters, V. 39, P. 1-1, 2018.
5. Lima, M. P.; Padilha, J. E.; Pontes, R. Borges; Fazzio, A.; Silva, A. J. R.
Stacking-Dependent Transport Properties in Few-Layers Graphene.
Solid State Communications, V. 250, P. 70-74, 2017.
6. Padilha, J. E.; Miwa, R. H.; da Silva, A. J. R.; Fazzio, A.
Two-Dimensional Van Der Waals P-N Junction of InSe/Phosphorene.
Physical Review B, V. 95, P. 195143, 2017.
7. Padilha, J. E.; Abdalla, L. B.; da Silva, A. J. R.; Fazzio, A.
Fully and Partially Iodinated Germanane as a Platform for the Observation of the Quantum Spin Hall Effect.
Physical Review B, V. 93, P. 045135-1-045135-6, 2016.
8. De Koning, M.; Fazzio, A.; da Silva, A. J. R.; Antonelli, A.
On the Nature of the Solvated Electron in Ice I_h.
Physical Chemistry Chemical Physics, V. 18, P. 4652-4658, 2016.
9. Padilha, J. E.; Janotti, A.; Fazzio, A.; da Silva, A. J. R.
Substrate-Supported Large-Band-Gap Quantum Spin Hall Insulator Based on III-V Bismuth Layers.
Physical Review B, V. 94, P. 195424, 2016.
10. Torres, A.; Pontes, R. Borges; da Silva, A. J. R.; Fazzio, A.
Tuning the thermoelectric Properties of a Single-Molecule Junction by Mechanical Stretching. Physical Chemistry Chemical Physics, V. 17, P. 5386-5392, 2015.
11. Padilha, J. E.; Fazzio, A.; da Silva, A. J. R.
Van Der Waals Heterostructure of Phosphorene and Graphene: Tuning the Schottky Barrier and Doping by Electrostatic Gating.
Physical Review Letters, V. 114, P. 066803, 2015.
12. Feliciano, Gustavo Troiano; da Silva, A. J. R.
Unravelling the Reaction Mechanism of Matrix Metalloproteinase Using QM/MM Calculations.
Journal of Molecular Structure, V. 1091, P. 125-132, 2015.
13. Acosta, C. M.; Lima, M. P.; Miwa, R. H.; da Silva, A. J. R.; Fazzio, A.
Topological Phases in Triangular Lattices of Ru Adsorbed on Graphene: Ab initio Calculations.
Physical Review. B, V. 89, P. 155438, 2014.
14. Padilha, Jose E.; Fazzio, A.; da Silva, A. J. R.

Directional Control of the Electronic and Transport Properties of Graphynes.
Journal of Physical Chemistry. C, V. 118, P. 18793-18798, 2014.

15. Torres, A.; Lima, M. P.; Fazzio, A.; da Silva, A. J. R.
Spin Caloritronics in Graphene With Mn.
Applied Physics Letters, V. 104, P. 072412-072412-4, 2014.
16. Souza, A. D.; Rungger, I.; Pontes, R. B.; Rocha, A. R.; da Silva, A. J. R.; Schwingenschlögl, U.; Sanvito, S.
Stretching of BDT-gold molecular junctions: thiol or thiolate termination?
Nanoscale, V. 6, P. 14495-14507, 2014.
17. Amorim, R. G.; Fazzio, A.; da Silva, A. J. R.; Rocha, A. R.
Confinement Effects and Why Carbon Nanotube Bundles Can Work as Gas Sensors.
Nanoscale, V. 5, P. 2798-2803, 2013.
18. Padilha, J. E.; Pontes, R. B.; da Silva, A. J. R.; Fazzio, A.
Graphene Nanoribbon intercalated With Hexagonal Boron Nitride: Electronic Transport
Properties From Ab initio Calculations.
Solid State Communications, V. 173, P. 24-29, 2013.
19. Almeida, J. M.; Rocha, A. R.; Singh, A. K.; da Silva, A. J. R.; Fazzio, A .
Electronic Transport in Patterned Graphene Nanoroads.
Nanotechnology, V. 24, P. 495201, 2013.
20. Lima, M. P.; Fazzio, A.; da Silva, A. J. R.
Interfaces Between Buckling Phases in Silicene: Ab initio Density Functional Theory
Calculations.
Physical Review. B, V. 88, P. 235413, 2013.
21. Padilha, J. E.; Seixas, L.; Pontes, R. B.; da Silva, A. J. R.; Fazzio, A.
Quantum Spin Hall Effect in a Disordered Hexagonal $\text{Si}_x\text{Ge}_{(1-x)}$ Alloy.
Physical Review. B, V. 88, P. 201106-1-201106-5, 2013.
22. Souza, A. M.; Fazzio, A.; da Silva, A. J. R.; Rocha, A. R.
Ab-initio Calculations for a Realistic Sensor: A Study of Co Sensors Based On Nitrogen-
Rich Carbon Nanotubes.
AIP Advances, V. 2, P. 032115-032115-8, 2012.
23. Feliciano, G. T.; da Silva, A. J. R.; Reguera, G.; Artacho, E.
Molecular and Electronic Structure of the Peptide Subunit of Conductive Pili From First
Principles.
The Journal of Physical Chemistry. A, V. 116, P. 8023-8030, 2012.
24. Padilha, J. E.; Amorim, R. G.; Rocha, A. R.; da Silva, A. J. R.; Fazzio, A.
Energetics and Stability of Vacancies in Carbon Nanotubes.
Solid State Communications, V. 151, P. 482-486, 2011.
25. Rigo, V. A.; Miwa, R H; da Silva, A. J. R.; Fazzio, A.
Mn Dimers on Graphene Nanoribbons: An Ab initio Study.

Journal of Applied Physics, V. 109, P. 053715-1-053715-4, 2011.

26. Almeida, J. M.; Rocha, A. R.; da Silva, A. J. R.; Fazzio, A.
Spin Filtering and Disorder-induced Magnetoresistance in Carbon Nanotubes: Ab initio Calculations.
Physical Review. B, V. 84, P. 085412-1-085412-6, 2011.
27. Padilha, J. E.; Lima, M. P.; da Silva, A. J. R.; Fazzio, A.
Bilayer Graphene Dual-Gate Nanodevice: an Ab initio Simulation.
Physical Review. B, V. 84, P. 113412-1-113412-4, 2011.
28. Lima, M. P.; da Silva, A. J. R.; Fazzio, A.
Adatoms in Graphene as A Source of Current Polarization: Role of the Local Magnetic Moment.
Physical Review. B, V. 84, P. 245411-1-245411-6, 2011.
29. Pontes, R. B.; Rocha, A. R.; Sanvito, S.; Fazzio, A; da Silva, A. J. R.
Ab initio Calculations of Structural Evolution and Conductance of Benzene-1,4-Dithiol on Gold Leads.
ACS Nano, V. 5, P. 795, 2011.
30. Padilha, J. E.; Pontes, R. B.; da Silva, A. J. R.; Fazzio, A.
IxV Curves of Boron and Nitrogen Doping Zigzag Graphene Nanoribbons.
International Journal of Quantum Chemistry, V. 111, P. 1379, 2011.
31. Lima, M. P.; da Silva, A. J. R.; Fazzio, A.
Splitting of the Zero-Energy Edge States in Bilayer Graphene.
Physical Review. B, V. 81, P. 045430, 2010.
32. Haas, P.; Tran, F.; Blaha, P.; Pedroza, L. S.; da Silva, A. J. R.; Odashima, M.; Capelle, K.
Systematic investigation of a Family of Gradient-Dependent Functionals for Solids.
Physical Review. B, V. 81, P. 125136, 2010.
33. da Silva, A. J. R.; Piquini, P.; Arantes, J. T.; Baierle, R. J.; Fazzio, A.
Mn-Doped Cubic Bn as an Atomiclike Memory Device: A Density Functional Study.
Physical Review. B, V. 81, P. 195432-1-195432-5, 2010.
34. Hobi Jr., E; Pontes, R. B.; Fazzio, A.; da Silva, A. J. R.
Formation of Atomic Carbon Chains From Graphene Nanoribbons.
Physical Review. B, V. 81, P. 201406-1-201406-4, 2010.
35. Rocha, A. R.; Martins, T. B.; Fazzio, A.; da Silva, A. J. R.
Disorder-Based Graphene Spintronics.
Nanotechnology, V. 21, P. 345202, 2010.
36. Rocha, A. R.; Rossi, M.; da Silva, A. J. R.; Fazzio, A.
Realistic Calculations of Carbon-Based Disordered Systems.
Journal of Physics. D, Applied Physics, V. 43, P. 374002, 2010.

37. Lima, M. P.; Rocha, A. R.; da Silva, A. J. R.; Fazzio, A.
Mimicking Nanoribbon Behavior Using a Graphene Layer on SiC.
Physical Review. B, V. 82, P. 153402-1-153402-4, 2010.
38. Correa, J. D.; da Silva, A. J. R.; Pacheco, M.
Tight-Binding Model for Carbon Nanotubes from Calculations.
Journal of Physics. Condensed Matter, V. 22, P. 275503, 2010.
39. Scopel, W L; Fazzio, A; da Silva, A. J. R.
Theoretical investigation of Hf and Zr Defects in C-Ge.
Journal of Physics. Condensed Matter, V. 21, P. 012206, 2009.
40. Rigo, V. A.; Martins, T. B.; da Silva, A. J. R.; Fazzio, A.; Miwa, R H.
Electronic, Structural, and Transport Properties of Ni-Doped Graphene Nanoribbons.
Physical Review B, V. 79, P. 075435, 2009.
41. Martins, T. B.; Fazzio, A.; da Silva, A. J. R.
Organic Molecule Assembled Between Carbon Nanotubes: A Highly Efficient Switch
Device.
Physical Review. B, V. 79, P. 115413, 2009.
42. Lima, M. P.; Fazzio, A; da Silva, A. J. R. .
Edge Effects in Bilayer Graphene Nanoribbons: Ab initio Total-Energy Density
Functional Theory Calculations.
Physical Review B, V. 79, P. 153401-1-153401-4, 2009.
43. Pedroza, L. S.; Capelle, K.; da Silva, A. J. R.
Gradient-Dependent Density Functionals of the Perdew-Burke-Ernzerhof Type for
Atoms, Molecules, and Solids.
Physical Review. B, V. 79, P. 201106(R), 2009.
44. E. Hobi Jr.; A. Fazzio; da Silva, A. J. R.
Temperature and Quantum Effects in the Stability of Pure and Doped Gold Nanowires.
Physical Review Letters, V. 100, P. 056104, 2008.
45. Pedroza, L. S.; da Silva, A. J. R.
Adiabatic intramolecular Movements for Water Systems.
The Journal of Chemical Physics, V. 128, P. 104311, 2008.
46. Rocha, A. R.; Padilha, J. E.; Fazzio, A; da Silva, A. J. R.
Transport Properties of Single Vacancies in Nanotubes.
Physical Review. B, V. 77, P. 153406, 2008.
47. Rocha, A. R.; Rossi, M; Fazzio, A; da Silva, A. J. R.
Designing Real Nanotube Based Gas Sensors (Editor's Suggestion).
Physical Review Letters, V. 100, P. 176803, 2008.
48. Scopel, W. L.; da Silva, A. J. R.; Fazzio, A.
Amorphous HfO₂ and HF_{1-x}Si_xO via a Melt-and-Quench Scheme Using Ab Initio
Molecular Dynamics.

Physical Review B, V. 77, P. 172101, 2008.

49. Martins, T. B.; Miwa, R. H.; da Silva, A. J. R.; Fazzio, A.
Sigma and Pi-Defects at Graphene Nanoribbon Edges: Building Spin Filters.
Nano Letters, V. 8, P. 2293-2298, 2008.
50. Pontes, R. B.; Silva, E. Z. da; Fazzio, A.; Silva, A. J. R.
Symmetry Controlled Spin Polarized Conductance in Au Nanowires.
Journal of the American Chemical Society, V. 130, P. 9897-9903, 2008.
51. Leão, C. R.; Fazzio, A.; da Silva, A. J. R.
Confinement and Surface Effects in B and P Doping of Silicon Nanowires.
Nano Letters, V. 8, P. 1866-1871, 2008.
52. Amorim, E. P. M.; da Silva, A. J. R.; da Silva, E. Z.
Computer Simulations of Copper and Gold Nanowires and Single-Wall Nanowires.
Journal of Physical Chemistry. C, V. 112, P. 15241-15246, 2008.
53. Arantes, J. T.; da Silva, A. J. R.; Fazzio, A; Antonelli, A.
Theoretical Investigation of A Mn-Doped Si/Ge Heterostructure.
Physical Review. B, V. 75, P. 075316, 2007.
54. Amorim, E. P. M.; da Silva, A. J. R.; Fazzio, A.; Silva, E. Z. da
Short Linear Atomic Chains in Copper Nanowires.
Nanotechnology, V. 18, P. 145701, 2007.
55. Arantes, J. T.; da Silva, A. J. R.; Fazzio, A.
Structural, Electronic, and Magnetic Properties of Mn-Doped Ge Nanowires by Ab initio
Calculations.
Physical Review B, V. 75, P. 115113, 2007.
56. Lima, M. P.; Pedroza, L. S.; da Silva, A. J. R.; Fazzio, A.; Vieira, D.; Freire, H. J. P.;
Capelle, K.
Simple Implementation of Complex Functionals: Scaled Self-Consistency.
Journal of Chemical Physics, V. 126, P. 144107, 2007.
57. Leão, C. R.; Fazzio, A.; da Silva, A. J. R.
Si Nanowires As Sensors: Choosing the Right Surface.
Nano Letters, V. 7, P. 1172, 2007.
58. Martins, T. B.; Miwa, R. H.; da Silva, A. J. R.; Fazzio, A.
Electronic and Transport Properties of Boron-Doped Graphene Nanoribbons.
Physical Review Letters, V. 98, P. 196803, 2007.
59. Scopel, W. L.; da Silva, A..J..R.; Fazzio, A.
Hf Defects in C-Si and their Importance for the HfO₂/Si Interface: Density-Functional
Calculations.
Physical Review B, V. 75, P. 193203, 2007.
60. Amorim, R. G.; Fazzio, A.; Antonelli, A.; Novaes, F. D.; da Silva, A. J. R.

Divacancies in Graphene and Carbon Nanotubes.
Nano Letters, V. 7, P. 2459-2462, 2007.

61. Pedroza, L. S.; da Silva, A. J .R.
Ab initio Monte Carlo Simulations Applied to a Si₅ Cluster.
Physical Review B - Condensed Matter and Materials Physics, V. 75, P. 245331, 2007.
62. Silva, E. Z. da; Novaes, F. D.; da Silva, A. J. R.; Fazzio, A.
Gold Nanowires and the Effect of Impurities.
Nanoscale Research Letters, V. 1, P. 91, 2006.
63. Novaes, F. D.; da Silva, A. J. R.; Silva, E. Z. da; Fazzio, A.
Oxygen Clamps in Gold Nanowires.
Physical Review Letters, V. 96, P. 016104, 2006.
64. Koning, M.; Antonelli, A.; da Silva, A. J. R.; Fazzio, A.
Orientational Defects in Ice Ih: An interpretation of Electrical Conductivity Measurements.
Physical Review Letters, V. 96, P. 075501, 2006.
65. Dalpian, G. M.; Wei, S. H.; Gong, X. G.; da Silva, A. J. R.; Fazzio, A.
Phenomenological Band Structure Model of Magnetic Coupling in Semiconductors.
Solid State Communications, V. 138, P. 353, 2006.
66. Zanella, I.; Fazzio, A.; da Silva, A. J. R.
C₅₉Si On the Monohydride Si(100):H-(2x1) Surface.
Journal of Physical Chemistry B, the, V. 110, P. 10849, 2006.
67. Pontes, R. B.; Novaes, F. D.; Fazzio, A.; da Silva, A. J. R.
Adsorption of Benzene-1,4-Dithiol On the Au(111) Surface and Its Possible Role in Molecular Conductance.
Journal of the American Chemical Society, V. 128, P. 8996, 2006.
68. Novaes, F. D.; da Silva, A. J. R.; Fazzio, A.
Density Functional theory Method for Non-Equilibrium Charge Transport Calculations:
Transampa.
Brazilian Journal of Physics, V. 36, P. 799-807, 2006.
69. Koning, M. de; Antonelli, A.; da Silva, A. J. R.; Fazzio, A.
Structure and Energetics of Molecular Point Defects in Ice Ih.
Physical Review Letters, V. 97, P. 155501-1-155501-4, 2006.
70. da Silva, A. J. R.; Fazzio, A.; Santos, R. R. dos; Oliveira, L. E.
Effects of Disorder On the Exchange Coupling in (Ga,Mn)As Diluted Magnetic Semiconductors.
Brazilian Journal of Physics, V. 36, P. 813-816, 2006.
71. Zanella, I.; Fazzio, A.; da Silva, A. J. R.
Electronic and Structural Properties of C₅₉Si on the Monohydride Si(100) Surface.
International Journal of Quantum Chemistry, V. 103, P. 557, 2005.

72. da Silva, A. J. R.; Fazzio, A.; Antonelli, A.
Bundling Up Carbon Nanotubes Through Wigner Defects.
Nano Letters, V. 5, P. 1045, 2005.
73. da Silva, A. J. R.; Fazzio, A.; Santos, R. R. dos; Oliveira, L. E.
Disorder and the Effective Mn-Mn Exchange interaction in $\text{Ga}_{1-x}\text{Mn}_x\text{As}$ Diluted Magnetic Semiconductors.
Physical Review. B, V. 72, P. 125208, 2005.
74. Hobi Jr., E.; da Silva, A. J. R.; Novaes, F. D.; Silva, E. Z. da; Fazzio, A.
Comment on “Contaminants in Suspended Gold Chains: An Ab initio Molecular Dynamics Study”.
Physical Review Letters, V. 95, P. 169601, 2005.
75. Novaes, F. D.; da Silva, A. J. R.; Fazzio, A.; Silva, E. Z. da
Computer Simulations in the Study of Gold Nanowires: the Effect of Impurities.
Applied Physics. A, Materials Science & Processing, V. 81, P. 1551, 2005.
76. Orellana, W.; da Silva, A. J. R.; Fazzio, A.
Oxygen-induced Atomic Desorptions in Oxynitrides: Density Functional Calculations.
Physical Review. B, V. 72, P. 205316, 2005.
77. Silva, E. Z. da; Novaes, F. D.; da Silva, A. J. R.; Fazzio, A.
Theoretical Study of the formation, Evolution, and Breaking of Gold Nanowires.
Physical Review. B, V. 69, P. 115411, 2004.
78. Scopel, W. L.; da Silva, A. J. R.; Orellana, W.; Fazzio, A.
Comparative Study of Defect Energetics in HfO_2 and SiO_2 .
Applied Physics Letters, V. 84, P. 1492, 2004.
79. Silva, E. Z. da; da Silva, A. J. R.; Fazzio, A.
Breaking of Gold Nanowires. Computational
Materials Science, V. 30, P. 73, 2004.
80. Fagan, S. B.; Mota, R.; da Silva, A. J. R.; Fazzio, A.
Substitutional Si Doping in Deformed Carbon Nanotubes.
Nano Letters, V. 4, P. 975, 2004.
81. Miranda, C. R.; Antonelli, A.; da Silva, A. J. R.; Fazzio, A.
Vacancy-Like Defects in a-Si: A First Principles Study.
Journal of Non-Crystalline Solids, V. 338340, P. 400, 2004.
82. Novaes, F. D.; Silva, E. Z. da; da Silva, A. J. R.; Fazzio, A.
Effect of Impurities on the Breaking of Au Nanowires.
Surface Science, V. 566568, P. 367, 2004.
83. Dalpian, G. M.; da Silva, A. J. R.; Fazzio, A.
Adsorption of Mn Atoms on the Si(100) Surface.
Surface Science, v. 566568, P. 688, 2004.

84. Fagan, S. B.; Mota, R.; da Silva, A. J. R.; Fazzio, A.
An Ab initio Study of Manganese Atoms and Wires interacting With Carbon Nanotubes.
Journal of Physics. Condensed Matter, V. 16, P. 3647, 2004.
85. Dalpian, G. M.; da Silva, A. J. R.; Fazzio, A.
Initial Stages of Ge and Si Growth Near Sb Monoatomic Steps On Si(100).
Physical Review. B, V. 70, P. 193306, 2004.
86. Orellana, W.; da Silva, A. J. R.; Fazzio, A.
Diffusion-Reaction Mechanisms of Nitriding Species in SiO₂.
Physical Review. B, V. 70, P. 125206, 2004.
87. da Silva, A. J. R.; Fazzio, A.; Antonelli, A.
Stabilization of Substitutional Mn in Silicon-Based Semiconductors.
Physical Review. B, V. 70, P. 193205, 2004.
88. da Silva, A. J. R.; Fazzio, A.; Santos, R. R. Dos; Oliveira, L. E.
First Principles Study of the Ferromagnetism in Ga_{1-x}Mn_xAs Semiconductors.
\Journal of Physics. Condensed Matter, V. 16, P. 8243, 2004.
89. Fagan, S. B.; Mota, R.; Baierle, R. J.; da Silva, A. J. R.; Fazzio, A.
Ab initio Study of an Organic Molecule interacting with a Silicon-Doped Carbon Nanotube.
Diamond and Related Materials, V. 12, P. 861, 2003.
90. Orellana, W.; da Silva, A. J. R.; Fazzio, A.
Oxidation at the Si/SiO₂ interface: influence of the Spin Degree of Freedom.
Physical Review Letters, V. 90, P. 016103, 2003.
91. Novaes, F. D.; da Silva, A. J. R.; Silva, E. Z. da; Fazzio, A.
Effect of Impurities in the Large Au-Au Distances in Gold Nanowires.
Physical Review Letters, V. 90, P. 036101, 2003.
92. Fagan, S. B.; da Silva, A. J. R.; Mota, R.; Baierle, R. J.; Fazzio, A.
Functionalization of Carbon Nanotubes Through the Chemical Binding of Atoms and Molecules.
Physical Review. B, V. 67, P. 033405, 2003.
93. Fagan, S. B.; Mota, R.; da Silva, A. J. R.; Fazzio, A.
Ab initio Study of An Iron Atom interacting With Single-Wall Carbon Nanotubes.
Physical Review. B, V. 67, P. 205414, 2003.
94. Fagan, S. B.; Mota, R.; Baierle, R. J.; da Silva, A. J. R.; Fazzio, A.
Energetics and Structural Properties of Adsorbed Atoms and Molecules on Silicon-Doped Carbon Nanotubes.
Materials Characterization, V. 50, P. 183, 2003.
95. Fagan, S. B.; Mota, R.; da Silva, A. J. R.; Fazzio, A.

Electronic and Magnetic Properties of Iron Chains on Carbon Nanotubes.
Microelectronics Journal, V. 34, P. 481, 2003.

96. Scopel, W. L.; da Silva, A. J. R.; Orellana, W.; Prado, R. J.; Fantini, M. C. A.; Fazzio, A.; Pereyra, I.
Theoretical and Experimental Studies of the Atomic Structure of Oxygen-Rich Amorphous Silicon Oxynitride Films.
Physical Review. B, V. 68, P. 155332, 2003.
97. Dalpian, G. M.; da Silva, A. J. R.; Fazzio, A.
Theoretical investigation of a Possible Mn_xSi_{1-x} Ferromagnetic Semiconductor.
Physical Review. B, V. 68, P. 113310, 2003.
98. da Silva, A. J. R.; Fazzio, A.; Santos, R. R. dos; Oliveira, L. E.
Electronic Structure and Origin of Ferromagnetism in $Ga_{1-x}Mn_xAs$ Semiconductors.
Physica B, V. 340342, P. 874, 2003.
99. Fagan, S. B.; Mota, R.; da Silva, A. J. R.; Fazzio, A.
Fe and Mn Atoms interacting With Carbon Nanotubes.
Physica B, V. 340342, P. 982, 2003.
100. Orellana, W.; da Silva, A. J. R.; Fazzio, A.
Influence of Spin State on Dynamical Processes of O_2 in Alfa-Quartz.
Materials Research Society, P. 32, 2002.
101. Venezuela, P.; Dalpian, G. M.; da Silva, A. J. R.; Fazzio, A.
Vacancy-Mediated Diffusion in Disordered Alloys: Ge Self-Diffusion in $Si_{1-x}Ge_x$.
Physical Review. B, V. 65, P. 193306, 2002.
102. Dalpian, G. M.; Venezuela, P.; da Silva, A. J. R.; Fazzio, A.
Ab initio Calculations of Vacancies in Si_xGe_{1-x} .
Applied Physics Letters, V. 81, P. 3383, 2002.
103. da Silva, A. J. R.; Baierle, R.; Mota, R.; Fazzio, A.
Native Defects in Germanium.
Physica B, V. 302303, P. 364, 2001.
104. Fagan, S. B.; Mota, R.; Baierle, R. J.; Paiva, G.; da Silva, A. J. R.; Fazzio, A.
Stability Investigation and Thermal Behavior of a Hypothetical Silicon Nanotube.
Journal of Molecular Structure. Theochem, V. 539, P. 101, 2001.
105. Dalpian, G. M.; Fazzio, A.; da Silva, A. J. R.
Adsorption of Monomers on Semiconductors and the Importance of the Surface Degrees of Freedom.
Physical Review. B, V. 63, P. 205303, 2001.
106. Dalpian, G. M.; Fazzio, A.; da Silva, A. J. R.
Theoretical STM Images of Ge Monomers and Trimers on Si(100).
Surface Science, V. 482485, P. 507, 2001.

107. da Silva, A. J. R.; Paz, O.; Sáenz, J. J.; Artacho, E.
Electron Correlation in the Si(100) Surface.
Surface Science, V. 482-485, P. 458-463, 2001.
108. da Silva, A. J. R.; Dalpian, G. M.; Janotti, A.; Fazzio, A.
Two-Atom Structures of Ge on Si(100): Dimers Versus Adatom Pairs.
Physical Review Letters, V. 87, P. 036104, 2001.
109. Baierle, R. J.; Fagan, S. B.; Mota, R.; da Silva, A. J. R.; Fazzio, A.
Electronic and Structural Properties of Silicon Doped Carbon Nanotubes.
Physical Review. B, V. 64, P. 085413, 2001.
110. Dalpian, G. M.; Fazzio, A.; da Silva, A. J. R.
Influence of Surface Degrees of Freedom on the Adsorption of Ge Ad-Atoms on Si(100).
Computational Materials Science, V. 22, P. 19, 2001.
111. Venezuela, P.; da Silva, A. J. R.; Silva, C.; Dalpian, G. M.; Fazzio, A.
Ab initio Studies of the $\text{Si}_{1-x}\text{Ge}_x$ Alloy and its intrinsic Defects.
Computational Materials Science, V. 22, P. 62, 2001.
112. Orellana, W.; da Silva, A. J. R.; Fazzio, A.
 O_2 Diffusion in SiO_2 : Triplet Versus Singlet.
Physical Review Letters, V. 87, P. 155901, 2001.
113. Venezuela, P.; Dalpian, G. M.; da Silva, A. J. R.; Fazzio, A.
Ab initio Determination of the Atomistic Structure of $\text{Si}_x\text{Ge}_{1-x}$ Alloy.
Physical Review. B, Condensed Matter, V. 64, P. 193202, 2001.
114. Silva, E. Z. da; da Silva, A. J. R.; Fazzio, A.
How Do Gold Nanowires Break?
Physical Review Letters, V. 87, P. 256102, 2001.
115. Silva, C.; Venezuela, P.; da Silva, A. J. R.; Fazzio, A.
Theoretical Investigation of the Pressure Induced Cubic-Diamond-Beta-Sn Phase Transition in the $\text{Si}_{0.5}\text{Ge}_{0.5}$.
Solid State Communications, V. 120, P. 369, 2001.
116. Fazzio, A.; Janotti, A.; da Silva, A. J. R.; Mota, R.
Microscopic Picture of the Single Vacancy in Germanium.
Physical Review. B, V. 61, P. R2401, 2000.
117. Fagan, S. B.; Baierle, R. J.; Mota, R.; da Silva, A. J. R.; Fazzio, A.
Ab initio Calculations for a Hypothetical Material: Silicon Nanotubes.
Physical Review. B, V. 61, P. 9994, 2000.
118. Azevedo, D. L.; da Silva, A. J. R.; Lima, M. A. P.
Effective Configurations in Electron-Molecule Scattering.
Physical Review. A, V. 61, P. 042702, 2000.
119. da Silva, A. J. R.; Janotti, A.; Fazzio, A.; Baierle, R. J.; Mota, R.

Self-interstitial Defect in Germanium.
Physical Review. B, V. 62, P. 9903, 2000.

120. Jarvis, E. A. A.; Fattal, E.; da Silva, A. J. R.; Carter, E. A.
Characterization of Photoionization Intermediates via Ab initio Molecular Dynamics.
The Journal of Physical Chemistry. A, V. 104, P. 2333, 2000.
121. Varella, M. T. N.; Bettega, M. H. F.; da Silva, A. J. R.; Lima, M. A. P.
Cross Sections for Rotational Excitations of NH₃, PH₃, AsH₃ and SbH₃ by Electron Impact.
The Journal of Chemical Physics, V. 110, P. 2452, 1999.
122. Janotti, A.; Baierle, R.; da Silva, A. J. R.; Mota, R.; Fazzio, A.
Electronic and Structural Properties of Vacancy and Self-interstitial Defects in Germanium.
Physica. B, Condensed Matter, V. 273274, P. 575, 1999.
123. Dalpian, G. M.; Janotti, A.; Fazzio, A.; da Silva, A. J. R.
Initial Stages of Ge Growth On Si(100): Ad-Atoms, Ad-Dimers and Ad-Trimmers.
Physica. B, Condensed Matter, V. 273274, P. 589, 1999.
124. da Silva, A. J. R.; Pang, J. W.; Carter, E. A.; Neuhauser, D.
Anharmonic Vibrations Via Filter Diagonalization of Ab initio Dynamics Trajectories.
The Journal of Physical Chemistry, V. 102, P. 881, 1998.
125. Govind, N.; Wang, Y. A.; da Silva, A. J. R.; Carter, E. A.
Accurate Ab initio Energetics of Extended Systems Via Explicit Correlation Embedded in a Density Functional Environment.
Chemical Physics Letters, V. 295, P. 129, 1998.
126. da Silva, A. J. R.; Cheng, H. Y.; Gibson, D. A.; Sorge, K. L.; Liu, Z.; Carter, E. A.
Limitations of Ab initio Molecular Dynamics Simulations of Simple Reactions: F + H₂ as a Prototype.
Spectrochimica Acta. Part A, Molecular Spectroscopy, V. A 53, P. 1285, 1997.
127. da Silva, A. J. R.; Radeke, M. R.; Carter, E. A.
Ab initio Molecular Dynamics of H₂ Desorption From Si(100)-2x1.
Surface Science, V. 381, P. L628, 1997.
128. da Silva, A. J. R.; Falicov, L. M.
Many-Body Calculation of the Magnetic, Optical and Charge-Transfer Spectra of the Solid Oxygen in the Alfa and Beta Phases.
Physical Review. B, V. 52, P. 2325, 1995.
129. da Silva, A. J. R.; Falicov, L. M.
Magnetism and the Alfa-Beta Phase Transition in Solid Oxygen.
Chemical Physics Letters, V. 222, P. 339, 1994.
130. Blase, X.; da Silva, A. J. R.; Zhu, X.; Louie, S.
Si 2p Core-Level Chemical Shifts at the H/Si(111)-(1×1) Surface.

Physical Review. B, V. 50, P. 8102-8105, 1994.

131. da Silva, A. J. R.; Falicov, L. M.

Calculation of Optical Transitions in NiI₂ and CoI₂ Under Pressure.

Physical Review. B, V. 45, P. 11511, 1992.

132. Skourtis, S. S.; da Silva, A. J. R.; Bialek, W.; Onuchic, J. N.

A New Look at the Primary Charge Separation in Bacterial Photosynthesis.

The Journal of Physical Chemistry, V. 96, P. 8034, 1992.

133. Lima, M. A. P.; Brescansin, L. M.; da Silva, A. J. R.; C. Winstead; Mckoy, V.

Applications of the Schwinger Multichannel Method of Electron-Molecule Collisions.

Physical Review. A, V. 41, P. 327, 1990.

134. da Silva, A. J. R.; Lima, M. A. P.; Brescansin, L. M.; Mckoy, V.

Schwinger Multichannel Method: A Study of a Feshbach Resonance in e-H₂ Collisions.

Physical Review. A, V. 41, P. 2903, 1990.