

Antonio José Roque da Silva

Articles

1. Fonseca, M. D.; Araujo, B. H. S.; Dias, C. S. B.; Archilha, N. L.; Neto, D. P. A.; Cavaleiro, 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 HfO_2 and $\text{HF}_{1-x}\text{Si}_x\text{O}$ 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 Ga_{1-x}Mn_xAs 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 HfO₂ and SiO₂.
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-Trimers.
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)-(1x1) 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.