

Publication List - Rodrigo B. Capaz

123. [*n-Diamondynes: Expanding the family of carbon allotropes*](#), D. G. Costa, F. J. F. S. Henrique, F. L. Oliveira, R. B. Capaz, and P. M. Esteves, *Carbon* 136, 337 (2018).
122. [*High hole-mobility of rrP3HT in organic field-effect transistors using low-polarity polyurethane gate dielectric*](#), H. C. Avila, P. Serrano, A. R. J. Barreto, Z. Ahmed, C. P. Gouvêa, C. Vilani, R. B. Capaz, C. F. N. Marchiori, M. Cremona, *Organic Electronics* 58, 33 (2018).
121. [*Linear magnetoresistivity in layered semimetallic \$\text{CaAl}_2\text{Si}_2\$*](#) , D. G. Costa, R. B. Capaz, R. Falconi, S. Strikos and M. ElMassalami, *Sci. Rep.* 8, 4102 (2018).
120. [*Tight binding parametrization of few-layer black phosphorus from first-principles calculations*](#), M. G. Menezes and R. B. Capaz, *Comp. Mater. Sci.* 143, 411 (2018).
119. [*Disentangling contributions of point and line defects in the Raman spectra of graphene-related materials*](#), L.G. Cançado, M. G. da Silva, E. H. Martins-Ferreira, F. Hof, K. Campiotti, K. Huang, A. Pénicaud, C. A. Achete, R. B. Capaz and A. Jorio, *2D Mater.* 4, 025039 (2017).
118. [*Giant and Tunable Anisotropy of Nanoscale Friction in Graphene*](#), C. M. Almeida, R. Prioli, B. Fragneaud, L. G. Cançado, R. Paupitz, D. S. Galvão, M. De Cicco, M. G. Menezes, C. A. Achete, and R. B. Capaz, *Sci. Rep.* 6, 31569 (2016).
117. [*Investigation of organic magnetoresistance dependence on spin-orbit coupling using 8-hydroxyquinolate rare-earth based complexes*](#), R. S. Carvalho, D. G. Costa, H. C. Ávila, T. B. Paolini, H. F. Brito, Rodrigo B. Capaz and M. Cremona, *Appl. Phys. Lett.* 108, 203303 (2016).
116. [*Boron-substitution and defects in B2-type AlNi compound: Site preference and influence on structural, thermodynamic and electronic properties*](#), R. B. Capaz, M. ElMassalami, L. A. Terrazos, M. Elhadi, H. Takeya, and L. Ghivelder, *J. Alloys Compd.* 669, 210-216 (2016).
115. [*Effects of edge magnetism on the Kohn anomalies of zigzag graphene nanoribbons*](#), F. J. Culchac and R. B. Capaz, *Nanotechnology* 27, 065707 (2016).
114. [*Donor wave functions in Si gauged by STM images*](#), A. L. Saraiva, J. Salfi, J. Bocquel, B. Voisin, S. Rogge, R. B. Capaz, M. J. Calderón, and B. Koiller, *Phys. Rev. B* 93, 045303 (2016).
113. [*Phosphorous bonding in single wall carbon nanotubes studied by X-ray photoelectron spectroscopy and DFT calculations*](#), J. R. Araujo, A. M. Silva, C. P. Gouvêa, E. S. Lopes, R. A. A. Santos, L. A. Terrazos, R. B. Capaz, C. A. Achete, I. O. Maciel, *Carbon* 99, 1 (2016).

112. [Electronic and structural properties of vacancies and hydrogen adsorbates on trilayer graphene](#), M. G. Menezes and R. B. Capaz, J. Phys.: Condens. Matter 27, 335302 (2015).
111. [Structural analysis of zeolite beta through periodic ab initio simulations of XRD and \$^{29}\text{Si}\$ and \$^{17}\text{O}\$ NMR spectra](#), D. G. Costa and R. B. Capaz, J. Mol. Struct. 1097, 112 (2015).
110. [Chemical Analysis and Molecular Models for Calcium–Oxygen–Carbon Interactions in Black Carbon Found in Fertile Amazonian Anthrosoils](#), B. S. Archanjo, J. R. Araujo, A. M. Silva, R. B. Capaz, N. P. S. Falcão, A. Jorio and C. A. Achete, Environ. Sci. Technol. 48, 7445-7452 (2014).
109. [Systematic determination of absolute cross-section of individual carbon nanotubes](#), K. Liu, X. Hong, S. Choi, C. Jin, R. B. Capaz, J. Kim, W. Wang, X. Bai, S. G. Louie, E. Wang and F. Wang, PNAS 111, 7564-7569 (2014).
108. [Magnetic response of zigzag nanoribbons under electric fields](#), F. J. Culchac, R. B. Capaz, A. T. Costa and A. Latgé, J. Phys.: Condens. Matter 26, 216002 (2014).
107. [Ab initio quasiparticle band structure of ABA and ABC-stacked graphene trilayers](#), M. G. Menezes, R. B. Capaz and S. G. Louie, Phys. Rev. B 89, 035431 (2014).
106. [Quantifying defects in N-layer graphene via a phenomenological model of Raman spectroscopy](#), R. Giro, B. S. Archanjo, E. H. M. Ferreira, R. B. Capaz, A. Jorio, and C. A. Achete, Nucl. Inst. Meth. Phys. Res. B 319, 71 (2014).
105. [Intermolecular interactions and substrate effects for an adamantane monolayer on a Au\(111\) surface](#), Y. Sakai, G. D. Nguyen, R. B. Capaz, S. Coh, I. V. Pechenezhskiy, X. Hong, F. Wang, M. F. Crommie, S. Saito, S. G. Louie and M. L. Cohen, Phys. Rev. B 88, 235407 (2013).
104. [A combined LEED and DFT surface structure determination of Cu₃Au\(001\): Evidence of a surface stacking fault](#), A. A. C. Cotta, D. V. P. Massote, G. A. S. Ribeiro, G. C. S. Valadares, R. B. Capaz, E. A. Soares e W. A. A. Macedo, Surf. Sci. 618, 167 (2013).
103. [Resonance effects on the Raman spectra of graphene superlattices](#), V. Carozo, C. M. Almeida, B. Fragneaud, P. M. Bedê, M. V. O. Moutinho, J. Ribeiro-Soares, N. F. Andrade, A. G. Souza Filho, M. J. S. Matos, B. Wang, M. Terrones, R. B. Capaz, A. Jorio, C. A. Achete, and L. G. Cançado, Phys. Rev. B 88, 085401 (2013).
102. [Probing the electronic properties of ternary \$A_nM_{3n-1}B_{2n}\$ \(\$n = 1\$: \$A = \text{Ca, Sr}\$; \$M = \text{Rh, Ir}\$ and \$n=3\$: \$A = \text{Ca, Sr}\$; \$M = \text{Rh}\$ \) phases: observation of superconductivity](#), H. Takeya, M. ElMassalami, L. A. Terrazos, R. E. Rapp, R. B. Capaz, H. Fujii, Y. Takano, M. Doerr, and S. A. Granovsky, Sci. Technol. Adv. Mater. 14, 035003 (2013).
101. [Molecular hyperfine fields in organic magnetoresistance devices](#), R. Giro, F. P. Rosselli, R. S. Carvalho, R. B. Capaz, M. Cremona and C. A. Achete, Phys. Rev. B 87, 125204 (2013).

100. [An Explicit Formula for Optical Oscillator Strength of Excitons in Semiconducting Single-Walled Carbon Nanotubes: Family Behavior](#), S. Choi, J. Deslippe, R. B. Capaz and S. G. Louie, Nano Lett. 13, 54 (2013).
99. [First-principles studies of oxygen-induced copper segregation in Cu₃Au\(111\)](#), A. M. Silva, C. A. Achete and R. B. Capaz, Chem. Phys. 410, 99 (2013).
98. [Effects of disorder range and electronic energy on the perfect transmission in graphene nanoribbons](#), L. R. F. Lima, F. A. Pinheiro, R. B. Capaz, C. H. Lewenkopf, E. R. Mucciolo, Phys. Rev. B 86, 205111 (2012).
97. [Half-metallicity induced by charge injection in hexagonal boron nitride clusters embedded in graphene](#), M. G. Menezes and R. B. Capaz, Phys. Rev. B 86, 195413 (2012).
96. [Structural determination of stable MoO_x monolayers on O/Cu₃Au\(100\): DFT calculations](#), G. C. S. Valadares, F. M. T. Mendes, M. D. Moreira, A. A. Leitão, H. Niehus, R. B. Capaz, C. A. Achete, Chem. Phys. 406, 47 (2012).
95. [Structural and phonon properties of bundled single- and double-wall carbon nanotubes under pressure](#), A. L. Aguiar, R. B. Capaz, A. G. Souza Filho, A. San-Miguel, J. Phys. Chem. C 116, 22637 (2012).
94. [Microscopic model of a phononic refrigerator](#), L. Arrachea, E. R. Mucciolo, C. Chamon, R. B. Capaz, Phys. Rev. B 86, 125424 (2012).
93. [Anomalous insulator-metal transition in boron nitride-graphene hybrid atomic layers](#), L. Song, L. Balicas, D. J. Mowbray, R. B. Capaz, K. Storr, L. Ci, D. Jariwala, S. Kurth, S. G. Louie, A. Rubio, P. M. Ajayan, Phys. Rev. B 86, 075429 (2012).
92. [Ab initio studies of pristine and oxidized Cu₃Au\(100\) and \(111\) surfaces](#), A. A. Leitão, M. D. Moreira, L. G. Dias, A. M. Silva, R. B. Capaz, C. A. Achete, J. Mater. Sci. 47, 7594 (2012).
91. [First-principles calculations and XPS measurements of gold segregation at the Cu₃Au\(111\) surface](#), M. D. Moreira, G. N. Fontes, H. Niehus, C. A. Achete, R. B. Capaz, J. Vac. Sci. Technol. B 30, 051802 (2012).
90. [An atlas of carbon nanotube optical transitions](#), K. Liu, J. Deslippe, F. Xiao, R. B. Capaz, X. Hong, S. Aloni, A. Zettl, W. Wang, X. Bai, S. G. Louie, E. Wang, and F. Wang, Nature Nanotech. 7, 325 (2012).
89. [Production and Characterization of Boron-Doped Single Wall Carbon Nanotubes](#), F. H. Monteiro, D. G. Larrude, M. E. H. Maia da Costa, L. A. Terrazos, R. B. Capaz, and F. L. Freire, Jr., J. Phys. Chem. C 116, 3281 (2012).
88. [Intervalley coupling for interface-bound electrons in silicon: An effective-mass study](#), A. L. Saraiva, M. J. Calderón, R. B. Capaz, X. Hu, S. Das Sarma, and Belita Koiller, Phys. Rev. B 84, 155320 (2011).

87. [Theory of magnetic edge states in chiral graphene nanoribbons](#), O. V. Yazyev, R. B. Capaz, and S. G. Louie, Phys. Rev. B 84, 115406 (2011).
86. [Quantifying defects in graphene via Raman spectroscopy at different excitation energies](#), L. G. Cançado, A. Jorio, E. H. Martins Ferreira, F. Stavale, C. A. Achete, R. B. Capaz, M. V. O. Moutinho, A. Lombardo, T. S. Kulmala, and A. C. Ferrari, Nano Lett. 11, 3190 (2011).
85. [Spatially resolving edge states of chiral graphene nanoribbons](#), C. Tao, L. Jiao, O. V. Yazyev, Y.-C. Chen, J. Feng, X. Zhang, R. B. Capaz, J. M. Tour, A. Zettl, S. G. Louie, H. Dai and M. F. Crommie, Nature Phys. 7, 616 (2011).
84. [Direct comparison between two \$\gamma\$ -alumina structural models by DFT calculations](#), A. R. Ferreira, M. J. F. Martins, E. Konstantinova, R. B. Capaz, Wladimir F. Souza, S. S. X. Chiaro, A. A. Leitão, J. Solid. State. Chem. 184, 1105 (2011).
83. [Heat pumping in nanomechanical systems](#), C. Chamon, E. R. Mucciolo, L. Arrachea and R. B. Capaz, Phys. Rev. Lett. 106, 135504 (2011).
82. [Hyperfine interactions in silicon quantum dots](#), L. Assali, H. Petrilli, R. B. Capaz, B. Koiller, S. Das Sarma and X. Hu, Phys. Rev. B 83, 165301 (2011).
81. [Pressure Induced Collapse in Double Wall Carbon Nanotubes: Chemical and Mechanical Screening Effects](#), A. Aguiar, E. B. Barros, R. B. Capaz, A. G. Souza Filho, P. Freire, J. Mendes Filho, D. Machon, C. Caillier, Y.-A. Kim, H. Muramatsu, M. Endo, A. San-Miguel, J. Phys. Chem. C, J. Phys. Chem. C 115, 5378 (2011).
80. [Properties of Charged Defects on Unidimensional Polymers](#), J. F. P. Leal, S. J. S. da Silva, E. R. Granhen, C. A. B. Silva Jr., M. Dionízio Moreira, C. A. Achete, R. B. Capaz and J. Del Nero, J. Comp. Theo. Nanoscience 8, 541 (2011).
79. [Gap opening by asymmetric doping in graphene bilayers](#), M. G. Menezes, R. B. Capaz, and J. L. B. Faria, Phys. Rev. B 82, 245414 (2010).
78. [Measuring disorder in graphene with the G and D bands](#), A. Jorio, E. H. Martins Ferreira, M. V. O. Moutinho, F. Stavale, C. A. Achete and R. B. Capaz, Phys. Stat. Sol (b)247, 2980 (2010).
77. [Evolution of the Raman spectra from single, few and many layers graphene with increasing disorder](#), E. H. Martins Ferreira, M. V. O. Moutinho, F. Stavale, M. M. Lucchese, R. B. Capaz, C. A. Achete and A. Jorio, Phys. Rev. B 82, 125429 (2010).
76. [Raman study of ion-induced defects in N-layer graphene](#), A. Jorio, M. M. Lucchese, F. Stavale, E. H. Martins Ferreira, M. V. O. Moutinho, R. B. Capaz and C. A. Achete, J. Phys.: Condens. Matter 22, 334204 (2010).
75. [Signatures of oxygen on Cu₃Au \(100\): From isolated impurity to oxide regimes](#), A. A. Leitão, L. G. Dias, M. Dionízio Moreira, F. Stavale, H. Niehus, C. A. Achete, and R. B. Capaz, Phys. Rev. B 82, 045408 (2010).

74. [*Comment on "Wave-scattering formalism for thermal conductance in thin wires with surface disorder"*](#), M. G. Menezes, J. Del Nero, R. B. Capaz and L. G. C. Rego, Phys. Rev. B 81, 117401 (2010).
73. [*Molecular Electronics Devices: A Short Review*](#), J. Del Nero, F. M. de Souza, and R. B. Capaz, J. Comput. Theor. Nanosci. 7, 503 (2010).
72. [*Quantifying ion-induced defects and Raman relaxation length in graphene*](#), M. M. Lucchese, F. Stavale, E. H. Martins Ferreira, C. Vilani, M. V. O. Moutinho, Rodrigo B. Capaz, C. A. Achete, and A. Jorio, Carbon 48, 1592 (2010).
71. [*Proposal for a single-molecule field-effect transistor for phonons*](#), M. G. Menezes, A. Saraiva-Souza, J. Del Nero, and R. B. Capaz, Phys. Rev. B 81, 012302 (2010).
70. [*Experimental and theoretical investigation of tris-\(8-hydroxy-quinolate\) aluminum \(Alq3\) photo degradation*](#), F. P. Rosselli, W. G. Quirino, C. Legnani, V. L. Calil, K. C. Teixeira, A. A. Leitão, R. B. Capaz, M. Cremona, C. A. Achete, Organic Electronics 10, 1417 (2009).
69. [*Charge transfer and screening effects in polyynes encapsulated inside single-wall carbon nanotubes*](#), L. G. Moura, L. M. Malard, M. A. Carneiro, P. Venezuela, Rodrigo B. Capaz, D. Nishide, Y. Achiba, H. Shinohara, and M. A. Pimenta, Phys. Rev. B 80, 161401(R) (2009).
68. [*Electron-hole interactions in carbon nanotubes: Novel Screening and exciton excitation spectra*](#), J. Deslippe, M. Dipoppa, D. Prendergast, M. V. O. Moutinho, R. B. Capaz and S. G. Louie, Nano Lett. 9, 1330 (2009).
67. [*Early Stages of Vanadium Deposition on Si\(111\)-7x7*](#), M. M. de Araújo, F. Stavale, A. A. Leitao, H. Niehus, C. A. Achete, and R. B. Capaz, Surf. Sci. 603, 835 (2009).
66. [*Quasiparticle and Excitonic Effects in the Optical Response of Nanotubes and Nanoribbons*](#), C. D. Spataru, S. Ismail-Beigi, R. B. Capaz, and S. G. Louie, em "Carbon Nanotubes", Ed.: A. Jorio, M. S. Dresselhaus e G. Dresselhaus, Springer, 2008, Top. Appl. Phys. 111, 195 (2008).
65. [*Resonance Raman study of polyynes encapsulated in single-wall carbon nanotubes*](#), L. M. Malard, D. Nishide, L. G. Dias, R. B. Capaz, A. P. Gomes, A. Jorio, C. A. Achete, R. Saito, Y. Achiba, H. Shinohara, and M. A. Pimenta, Phys. Rev. B 76, 233412 (2007).
64. [*Chemical identification in the Cu₃Au\(100\) surface using scanning tunneling microscopy and first-principles calculations*](#), L. G. Dias, A. A. Leitão, C. A. Achete, R.-P. Blum, H. Niehus, R. B. Capaz, Surf. Sci. 601, 5540 (2007).
63. [*Excitons in carbon nanotubes: Diameter and chirality trends*](#), R. B. Capaz, C. D. Spataru, S. Ismail-Beigi, and S. G. Louie, phys. stat. sol. (b) 244, 4016 (2007).

62. [Effect of post-growth annealing on the optical properties of InAs/GaAs quantum dots: A tight-binding study](#), R. Santoprete, P. Kratzer, M. Scheffler, R. B. Capaz, B. Koiller, J. Appl. Phys., 102, 023711 (2007).
61. [Straight to the bar: Molecular nanostructures, graphene, nanotubes](#), R. B. Capaz, Phys. Stat. Solidi (RRL) 1, A47 (2007).
60. [Diameter and chirality dependence of exciton properties in carbon nanotubes](#), R. B. Capaz, C. D. Spataru, S. Ismail-Beigi, and S. G. Louie, Phys. Rev. B 74, 121401 (2006).
59. [Review on the symmetry-related properties of carbon nanotubes](#), E. B. Barros, A. Jorio, Ge. G. Samsonidze, R. B. Capaz, A. G. Souza Filho, J. Mendes Filho, G. Dresselhaus and M. S. Dresselhaus, Phys. Rep. **431**, 261 (2006).
58. [Selection rules for one- and two-photon absorption by excitons in carbon nanotubes](#), E. B. Barros, R. B. Capaz, A. Jorio, Ge. G. Samsonidze, A. G. Souza Filho, S. Ismail-Beigi, C. D. Spataru, S. G. Louie, G. Dresselhaus, and M. S. Dresselhaus, Phys. Rev. B **73**, 241206 (2006).
57. [Temperature dependence of the optical transition energies of carbon nanotubes: The role of electron-phonon coupling and thermal expansion](#), S. B. Cronin, Y. Yin, A. Walsh, R. B. Capaz, A. Stolyarov, P. Tangney, M. L. Cohen, S. G. Louie, A. K. Swan, M. S. Unlu, B. B. Goldberg, and M. Tinkham, Phys. Rev. Lett. **96**, 127403 (2006).
56. [Application of standard DFT theory for nonbonded interactions in soft matter: Prototype study of poly-para-phenylene](#), M. Alves-Santos, L. Y. A. Dávila, H. M. Petrilli, R. B. Capaz, and M. J. Caldas, J. Comp. Chem. **27**, 217 (2006).
55. [Theory and Ab Initio Calculation of Radiative Lifetime of Excitons in Semiconducting Carbon Nanotubes](#), C. D. Spataru, S. Ismail-Beigi, R. B. Capaz, and S. G. Louie, Phys. Rev. Lett. **95**, 247402 (2005).
54. [Structural transformations of carbon nanotubes under hydrostatic pressure](#), P. Tangney, R. B. Capaz, C. D. Spataru, M. L. Cohen, and S. G. Louie, Nano Lett. **5**, 2268 (2005).
53. [Silicon-based spin and charge quantum computation](#), B. Koiller, X. D. Hu, R. B. Capaz, A. S. Martins, and S. Das Sarma, An. Acad. Bras. Ciênc. **77**, 201 (2005).
52. [Theory of sodium ordering in \$Na_xCoO_2\$](#) , P. H. Zhang, R. B. Capaz, M. L. Cohen, and S. G. Louie, Phys. Rev. B **71**, 153102 (2005).
51. [Resonance Raman spectroscopy \(n,m\)-dependent effects in small-diameter single-wall carbon nanotubes](#), A. Jorio, C. Fantini, M. A. Pimenta, R. B. Capaz, Ge. G. Samsonidze, G. Dresselhaus, M. S. Dresselhaus, J. Jiang, N. Kobayashi, A. Grüneis, and R. Saito, Phys. Rev. B **71**, 075401 (2005).

50. [*Temperature dependence of the band gap of semiconducting carbon nanotubes*](#), R. B. Capaz, C. D. Spataru, P. Tangney, M. L. Cohen, and S. G. Louie, Phys. Rev. Lett. **94**, 036801 (2005).
49. [*Hydrostatic pressure effects on the structural and electronic properties of carbon nanotubes*](#), R. B. Capaz, C. D. Spataru, P. Tangney, M. L. Cohen, and S. G. Louie, phys. stat. sol. (b) **214**, 3352 (2004), Proceedings of The 11th International Conference on High Pressure Semiconductor Physics, August 2-5 2004, Berkeley (CA), USA.
48. [*Shallow-donor wave functions and donor-pair exchange in silicon: Ab initio theory and floating-phase Heitler-London approach*](#), B. Koiller, R. B. Capaz, X. Hu, and S. Das Sarma, Phys. Rev. B **70**, 115207 (2004).
47. [*Group-V mixing effects in the structural and optical properties of \$\(\text{ZnSi}\)_{1/2}\text{P}_{1/4}\text{As}_{3/4}\$*](#) , A. A. Leitão and R. B. Capaz, Phys. Rev. B **70**, 085207 (2004).
46. [*Electric-field control and adiabatic evolution of shallow donor impurities in silicon*](#), A. S. Martins, R. B. Capaz, and B. Koiller, Phys. Rev. B **69**, 085320 (2004).
45. [*Tight-binding study of the influence of the strain on the electronic properties of InAs/GaAs quantum dots*](#), R. Santoprete, B. Koiller, R. B. Capaz, P. Kratzer, Q. K. K. Liu and M. Scheffler, Phys. Rev. B **68**, 235311 (2003).
44. [*Mixed-oxide formation during preparation of alumina-supported zirconia: an EXAFS and DFT study*](#), A. C. Faro, K. R. Souza, J. G. Eon, A. A. Leitão, A. B. Rocha, and R. B. Capaz, Phys. Chem. Chem. Phys. **5** (17), 3811-3817 (2003).
43. [*Ab initio calculations of structural and dynamical properties of poly\(p-phenylene\) and poly\(p-phenylene vinylene\)*](#), R. B. Capaz and M. J. Caldas, Phys. Rev. B **67**, 205205 (2003).
42. [*Electromechanical effects in carbon nanotubes: Ab initio and analytical tight-binding calculations*](#), M. Veríssimo-Alves, B. Koiller, H. Chacham, and R. B. Capaz, Phys. Rev. B **67**, 161401 (2003).
41. [*Switching times in electric-field-tunable GaAs/AlAs heterostructures*](#), F. J. Ribeiro, R. B. Capaz, and B. Koiller, Appl. Phys. Lett. **81**, 2247 (2002).
40. [*Atomistic description of shallow levels in semiconductors*](#), A. S. Martins, J. G. Menchero, R. B. Capaz, and B. Koiller, Phys. Rev. B **65**, 245205 (2002).
39. [*Electric-field effects on the band-edge states of GaAs/AlAs coupled quantum wells*](#), F. J. Ribeiro, R. B. Capaz, and B. Koiller, phys. stat. sol. (b) **232**, 148 (2002) - Proceedings of Nano 2001: 2nd Ibero American Workshop on Nanostructures for Application in Micro and Optoelectronics, November 2001, São José dos Campos, Brazil.
38. [*The nature of shallow-state wave functions in semiconductors*](#), A. S. Martins, J. G. Menchero, R. B. Capaz, and B. Koiller, phys. stat. sol. (b) **232**, 106 (2002) - Proceedings of Nano 2001: 2nd Ibero American Workshop on Nanostructures for

Application in Micro and Optoelectronics, November 2001, São José dos Campos, Brazil.

37. [Electric-field effects on the band-edge states of GaAs/AlAs coupled quantum wells](#), F. J. Ribeiro, R. B. Capaz, and B. Koiller, *Braz. J. Phys.* **32**, 318 (2002) - Proceedings of the 10th Brazilian Workshop on Semiconductor Physics, April 2001, Guarujá, Brazil.

36. [Ab initio studies of electromechanical effects in carbon nanotubes](#), M. Veríssimo-Alves, R. B. Capaz, B. Koiller, E. Artacho, and H. Chacham, *Braz. J. Phys.* **32**, 427 (2002), Proceedings of the 10th Brazilian Workshop on Semiconductor Physics, April 2001, Guarujá, Brazil.

35. [Comment on "Polarons in Carbon Nanotubes": Reply](#), M. Veríssimo-Alves, R. B. Capaz, B. Koiller, H. Chacham, and E. Artacho, *Phys. Rev. Lett.* **89**, 049702 (2002).

34. [Hyperfine interactions and lattice distortion of the F center in KCl, NaCl and LiCl crystals](#), A. A. Leitão, R. B. Capaz, N. V. Vugman, and C. E. Bielschowsky, *J. Mol. Struct.: Theochem* **580**, 65 (2002), Proceedings of the X *Simpósio Brasileiro de Química Teórica*, November 1999, Caxambu, Brazil.

33. [Ab initio study of atomic oxygen adsorption on the Si\(111\)7 x 7 surface](#), M. J. Caldas, R. J. Baierle, R. B. Capaz, and E. Artacho, *Physica B* **308**, 329 (2001), Proceedings of the 21st International Conference on Defects in Semiconductors, July 16-20 2001, Giessen, Germany.

32. [Ab-initio study of Coulomb-correlated optical properties in conjugated polymers](#), A. Ruini, F. Rossi, U. Hohenester, E. Molinari, R. B. Capaz, and M. J. Caldas, *Synth. Met.* **119**, 257 (2001), Proceedings of the 2000 International Conference on Science and Technology of Synthetic Metals, July 2000, Bad Gastein, Austria.

31. [Interface modulation and quantum well to quantum wire crossover in semiconductor heterostructures](#), T. G. Dargam, R. B. Capaz, and B. Koiller, *Phys. Rev. B* **64**, 245327 (2001).

30. [Polarons in Carbon Nanotubes](#), M. Veríssimo-Alves, R. B. Capaz, B. Koiller, E. Artacho, and H. Chacham, *Phys. Rev. Lett.* **86**, 3372 (2001).

29. [An elastic model for the In-In correlations in In_xGa_{1-x}As semiconductor alloys](#), A. S. Martins, B. Koiller, and R. B. Capaz, *Solid State Commun.* **115**, 287 (2000).

28. [Tight-binding total-energy method applied to polyacetylene](#), D. E. Tuyenrot, B. Koiller, and R. B. Capaz, *Phys. Rev. B* **61**, 7187 (2000).

27. [Quantum well to quantum wire crossover in AlAs/GaAs/AlAs heterostructures induced by interface roughness increase](#), T. G. Dargam, R. B. Capaz, and B. Koiller, *Braz. J. Phys.* **29**, 834 (1999), Proceedings of the 9th Brazilian Workshop on Semiconductor Physics, February 1999, Belo Horizonte, Brazil.

26. [Vacancy diffusion in silicon: analysis of transition state theory](#), R. R. Gattass, B. Koiller, and R. B. Capaz, Braz. J. Phys. **29**, 828 (1999), Proceedings of the 9th Brazilian Workshop on Semiconductor Physics, February 1999, Belo Horizonte, Brazil.
25. [Ab initio studies of hydrogen-enhanced oxygen diffusion in silicon](#), R. B. Capaz, L. V. C. Assali, L. C. Kimerling, K. Cho, and J. D. Joannopoulos, Braz. J. Phys. **29**, 611 (1999), Proceedings of the 9th Brazilian Workshop on Semiconductor Physics, February 1999, Belo Horizonte, Brazil.
24. [Density-functional and plane-wave approach to structural properties of poly\(p-phenylene\) and poly\(p-phenylene vinylene\)](#), R. B. Capaz and M. J. Caldas, J. Mol. Struct. (Theochem) **464**, 31 (1999), Proceedings of the IX Simpósio Brasileiro de Química Teórica, November 1997, Caxambu, Brazil.
23. [Semiconductor heterostructures with non-ideal interfaces: electronic structure and optical properties](#), R. B. Capaz, T. G. Dargam, A. S. Martins, B. Koiller, and H. Chacham, phys. stat. sol. (a) **173**, 235 (1999), Proceedings of the 2nd German-Brazilian Workshop on Applied Surface Science, September 1998, Templin, Germany.
22. [Role of interface imperfections on intervalley coupling in GaAs/AlAs superlattices](#), J. G. Menchero, B. Koiller, and R. B. Capaz, Phys. Rev. Lett. **83**, 2034 (1999).
21. [Segregation, interface morphology, and the optical properties of GaAs/AlAs quantum wells: A theoretical study](#), B. Koiller, R. B. Capaz, and H. Chacham, Phys. Rev. B. **60**, 1787 (1999).
20. [Mechanism for hydrogen-enhanced oxygen diffusion in silicon](#), R. B. Capaz, L. V. C. Assali, L. C. Kimerling, K. Cho, and J. D. Joannopoulos, Phys. Rev. B **59**, 4898 (1999).
19. [Tight-binding scheme for impurity states in semiconductors](#), J. G. Menchero, R. B. Capaz, B. Koiller, and H. Chacham, Phys. Rev. B **59**, 2722 (1999).
18. *Atomic segregation and the optical properties of GaAs/AlAs heterostructures*, B. Koiller, R. B. Capaz, and H. Chacham, Rev. Mex. Fís. **44**, Supl. 3, 150 (1998), Proceedings of the XIV Simposio Latinoamericano de Física del Estado Sólido, January 1998, Oaxaca, Mexico.
17. [Theory of carbon-carbon pairs in silicon](#), R. B. Capaz, A. Dal Pino Jr., and J. D. Joannopoulos, Phys. Rev. B **58**, 9845 (1998).
16. [Critical analysis of the virtual crystal approximation](#), T. G. Dargam, R. B. Capaz, and B. Koiller, Braz. J. Phys. **27/A**, 299 (1997), Proceedings of the 8th Brazilian Workshop on Semiconductor Physics, February 1997, Águas de Lindóia, Brazil.
15. [Disorder and size effects in the envelope function approximation](#), T. G. Dargam, R. B. Capaz, and B. Koiller, Phys. Rev. B **56**, 9625 (1997).

14. [Unified approach for the calculation of force constants and accelerated convergence of atomic coordinates](#), R. B. Capaz, and J. D. Joannopoulos, Phys. Rev. B **54**, 13393 (1996).
13. [Ab initio studies of adatom vacancies on the Si\(111\)-\(7x7\) surface](#), H. Lim, K. Cho, R. B. Capaz, J. D. Joannopoulos, K. D. Brommer, and B. E. Larson, Phys. Rev. B **53**, 15421 (1996).
12. [Signatures of bulk and surface arsenic antisite defects in GaAs\(110\)](#), R. B. Capaz, K. Cho, and J. D. Joannopoulos, Phys. Rev. Lett. **75**, 1811 (1995).
11. [Ab initio studies of GaN epitaxial growth on SiC](#), R. B. Capaz, H. Lim, and J. D. Joannopoulos, Phys. Rev. B **51**, 17755 (1995).
10. [Direct-to-indirect crossover in semiconductor alloys: A first-order phase transition?](#), B. Koiller and R. B. Capaz, Phys. Rev. Lett. **74**, 769 (1995).
9. [Manifestation of quantum chaos in electronic band structures](#), E. R. Mucciolo, R. B. Capaz, B. L. Altshuler, and J. D. Joannopoulos, Phys. Rev. B **50**, 8245 (1994).
8. [Identification of the migration path of interstitial carbon in silicon](#), R. B. Capaz, A. Dal Pino Jr., and J. D. Joannopoulos, Phys. Rev. B **50**, 7439 (1994).
7. *Gap properties of semiconductor alloys*, R. B. Capaz and B. Koiller, Braz. J. Phys. **23**, 161 (1993), Proceedings of the *Workshop on Crystalline and Amorphous Silicon and its Alloys*, May 27-29, 1992, Campinas, Brazil.
6. [Pressure and composition effects on the gap properties of \$Al_xGa_{1-x}As\$](#) , R. B. Capaz, G. C. de Araújo, B. Koiller, and J. P. von der Weid, J. Appl. Phys. **74**, 5531 (1993).
5. [Partial ordering effects in \$In_xGa_{1-x}P\$](#) , R. B. Capaz and B. Koiller, Phys. Rev. B **47**, 4044 (1993).
4. [Physical criteria for the direct-to-indirect gap crossover in \$Al_xGa_{1-x}As\$ alloys](#), R. B. Capaz, J. P. von der Weid, and B. Koiller, Appl. Phys. Lett. **60**, 704 (1992).
3. [Walks and polymers in two dimensions: dependence of the amplitudes on the valence angle](#), R. B. Capaz and C. M. Chaves, Phys. Rev. B **44**, 2366 (1991).
2. [Gap states and localization properties of 1-D Fibonacci quasicrystals](#), R. B. Capaz, B. Koiller, and S. L. A. Queiroz, Phys. Rev. B **42**, 6402 (1990).
1. [Growth-driven ordering and anisotropy in semiconductor alloys](#), R. B. Capaz, G. F. Preger, and B. Koiller, Phys. Rev. B **40**, 8299 (1989).