

**RODRIGO BARBOSA CAPAZ**  
Brazilian Nanotechnology National Laboratory  
Brazilian Center for Research in Energy and Materials

## **EDUCATION**

---

**PONTIFÍCIA UNIVERSIDADE CATÓLICA DO RIO DE JANEIRO**

B.S. Physics, December 1989

**PONTIFÍCIA UNIVERSIDADE CATÓLICA DO RIO DE JANEIRO**

M.S. Physics, June 1991

Thesis: *Pressure and Composition Effects in the Gap Properties of  $Al_xGa_{1-x}As$*

**MASSACHUSETTS INSTITUTE OF TECHNOLOGY**

Ph.D. Physics, June 1996

Thesis: *Ab Initio Studies of Semiconductors: Defects, Surfaces and Interfaces*

## **WORK EXPERIENCE**

---

- 2021-2024 **Brazilian Nanotechnology National Laboratory, Brazilian Center for Research in Energy and Materials**  
*Director*
  
- 1997-2021 **Instituto de Física, Universidade Federal do Rio de Janeiro**  
*Full Professor*
  - Research activities in theoretical physics of condensed matter and nanostructured systems
  - Undergraduate and graduate teaching
  - Visiting scholar at U. C. Berkeley (Physics Department) – 2004 and 2010

## **HONORS AND AWARDS**

---

- John Simon Guggenheim Memorial Foundation Fellowship – 2003
- “Young Scientist” Prize - Physics, TWAS-ROLAC, 2009
- Research Fellow 1A (highest rank) of the Brazilian Council of Research (CNPq)
- Member of the Brazilian Academy of Sciences
- President of the Brazilian Physical Society (2023-2025)

## **BIBLIOMETRICS (Google Scholar)**

---

- 164 articles
- 13,809 citations
- h-index = 45

## ARTICLES

---

1. *Growth-driven ordering and anisotropy in semiconductor alloys*, R. B. Capaz, G. F. Preger e B. Koiller, Phys. Rev. B **40**, 8299 (1989).
2. *Gap states and localization properties of 1-D Fibonacci quasicrystals*, R. B. Capaz, B. Koiller e S. L. A. Queiroz, Phys. Rev. B **42**, 6402 (1990).
3. *Walks and polymers in two dimensions: dependence of the amplitudes on the valence angle*, R. B. Capaz e C. M. Chaves, Phys. Rev. B **44**, 2366 (1991).
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 e B. Koiller, Appl. Phys. Lett. **60**, 704 (1992).
5. *Partial ordering effects in  $In_xGa_{1-x}P$* , R. B. Capaz e B. Koiller, Phys. Rev. B **47**, 4044 (1993).
6. *Pressure and composition effects on the gap properties of  $Al_xGa_{1-x}As$* , R. B. Capaz, G. C. de Araújo, B. Koiller e J. P. von der Weid, J. Appl. Phys. **74**, 5531 (1993).
7. *Gap properties of semiconductor alloys*, R. B. Capaz e 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.
8. *Identification of the migration path of interstitial carbon in silicon*, R. B. Capaz, A. Dal Pino Jr. e J. D. Joannopoulos, Phys. Rev. B **50**, 7439 (1994).
9. *Manifestation of quantum chaos in electronic band structures*, E. R. Mucciolo, R. B. Capaz, B. L. Altshuler e J. D. Joannopoulos, Phys. Rev. B **50**, 8245 (1994).
10. *Direct-to-indirect crossover in semiconductor alloys: A first-order phase transition?*, B. Koiller e R. B. Capaz, Phys. Rev. Lett. **74**, 769 (1995).
11. *Ab initio studies of GaN epitaxial growth on SiC*, R. B. Capaz, H. Lim e J. D. Joannopoulos, Phys. Rev. B **51**, 17755 (1995).
12. *Signatures of bulk and surface arsenic antisite defects in GaAs(110)*, R. B. Capaz, K. Cho e J. D. Joannopoulos, Phys. Rev. Lett. **75**, 1811 (1995).
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 e B. E. Larson, Phys. Rev. B **53**, 15421 (1996).
14. *Unified approach for the calculation of force constants and accelerated convergence of atomic coordinates*, R. B. Capaz e J. D. Joannopoulos, Phys. Rev. B **54**, 13393 (1996).
15. *Disorder and size effects in the envelope function approximation*, T. G. Dargam, R. B. Capaz e B. Koiller, Phys. Rev. B **56**, 9625 (1997).
16. *Critical analysis of the virtual crystal approximation*, T. G. Dargam, R. B. Capaz e B. Koiller, Braz. J. Phys. **27/A**, 299 (1997) – Proceedings of the *8<sup>th</sup> Brazilian Workshop on Semiconductor Physics*, February 1997, Águas de Lindóia, Brazil.
17. *Theory of carbon-carbon pairs in silicon*, R. B. Capaz, A. Dal Pino Jr., e J. D. Joannopoulos, Phys. Rev. B **58**, 9845 (1998).
18. *Atomic segregation and the optical properties of GaAs/AlAs heterostructures*, B. Koiller, R. B. Capaz e H. Chacham, Rev. Mex. Fís. **44**, Supl. 3, 150 (1998) – Proceedings of the *XIV Simposio Latinoamericano de Física del Estado Sólido*, January 1998, Oaxaca, México.
19. *Tight-binding scheme for impurity states in semiconductors*, J. G. Menchero, R. B. Capaz, B. Koiller e H. Chacham, Phys. Rev. B **59**, 2722 (1999).
20. *Mechanism for hydrogen-enhanced oxygen diffusion in silicon*, R. B. Capaz, L. V. C. Assali, L. C. Kimerling, K. Cho e J. D. Joannopoulos, Phys. Rev. B **59**, 4898 (1999).
21. *Segregation, interface morphology, and the optical properties of GaAs/AlAs quantum wells: A theoretical study*, B. Koiller, R. B. Capaz e H. Chacham, Phys. Rev. B **60**, 1787 (1999).
22. *Role of interface imperfections on intervalley coupling in GaAs/AlAs superlattices*, J. G. Menchero, B. Koiller e R. B. Capaz, Phys. Rev. Lett. **83**, 2034 (1999).
23. *Semiconductor heterostructures with non-ideal interfaces: electronic structure and optical properties*, R. B. Capaz, T. G. Dargam, A. S. Martins, B. Koiller e H. Chacham, phys. stat. sol. (a) **173**, 235 (1999) – Proceedings of the *2<sup>nd</sup> German-Brazilian Workshop on Applied Surface Science*, September 1998, Templin, Germany.
24. *Density-functional and plane-wave approach to structural properties of poly(p-phenylene) and poly(p-phenylene vinylene)*, R. B. Capaz e M. J. Caldas, J. Mol. Struct. (Theochem) **464**, 31 (1999) – Proceedings of the *IX Simpósio Brasileiro de Química Teórica*, November 1997, Caxambu, Brazil.

25. *Ab initio studies of hydrogen-enhanced oxygen diffusion in silicon*, R. B. Capaz, L. V. C. Assali, L. C. Kimerling, K. Cho e J. D. Joannopoulos, *Braz. J. Phys.* **29**, 611 (1999) – Proceedings of the 9<sup>th</sup> *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 e R. B. Capaz, *Braz. J. Phys.* **29**, 828 (1999) – Proceedings of the 9<sup>th</sup> *Brazilian Workshop on Semiconductor Physics*, February 1999, Belo Horizonte, Brazil.
27. *Quantum well to quantum wire crossover in AlAs/GaAs/AlAs heterostructures induced by interface roughness increase*, T. G. Dargam, R. B. Capaz e B. Koiller, *Braz. J. Phys.* **29**, 834 (1999) – Proceedings of the 9<sup>th</sup> *Brazilian Workshop on Semiconductor Physics*, February 1999, Belo Horizonte, Brazil.
28. *Tight-binding total-energy method applied to polyacetylene*, D. E. Tuyarot, B. Koiller, e R. B. Capaz, *Phys. Rev. B* **61**, 7187 (2000).
29. *An elastic model for the In-In correlations in In<sub>x</sub>Ga<sub>1-x</sub>As semiconductor alloys*, A. S. Martins, B. Koiller e R. B. Capaz, *Solid State Commun.* **115**, 287 (2000).
30. *Polarons in Carbon Nanotubes*, M. Verissimo-Alves, R. B. Capaz, B. Koiller, E. Artacho e H. Chacham, *Phys. Rev. Lett.* **86**, 3372 (2001).
31. *Interface modulation and quantum well to quantum wire crossover in semiconductor heterostructures*, T. G. Dargam, R. B. Capaz e B. Koiller, *Phys. Rev. B* **64**, 245327 (2001).
32. *Ab-initio study of Coulomb-correlated optical properties in conjugated polymers*, A. Ruini, F. Rossi, U. Hohenester, E. Molinari, R. B. Capaz e 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.
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 e E. Artacho, *Physica B* **308**, 329 (2001) – Proceedings of the 21<sup>st</sup> *International Conference on Defects in Semiconductors*, July 16-20, 2001, Giessen, Germany.
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 e C. E. Bielschowsky, *J. Mol. Struct. – Theochem* **580**, 65 (2002) – Proceedings of the X *Simpósio Brasileiro de Química Teórica*, November 1999, Caxambu, Brazil.
35. *Ab initio studies of electromechanical effects in carbon nanotubes*, M. Verissimo-Alves, R. B. Capaz, B. Koiller, E. Artacho e H. Chacham, *Braz. J. Phys.* **32**, 427 (2002) – Proceedings of the 10<sup>th</sup> *Brazilian Workshop on Semiconductor Physics*, April 2001, Guarujá, Brazil.
36. *Electric-field effects on the band-edge states of GaAs/AlAs coupled quantum wells*, F. J. Ribeiro, R. B. Capaz e B. Koiller, *Braz. J. Phys.* **32**, 318 (2002) - Proceedings of the 10<sup>th</sup> *Brazilian Workshop on Semiconductor Physics*, April 2001, Guarujá, Brazil.
37. *The nature of shallow-state wave functions in semiconductors*, A. S. Martins, J. G. Menchero, R. B. Capaz e B. Koiller, *phys. stat. sol. (b)* **232**, 106 (2002) - Proceedings of *Nano 2001: 2<sup>nd</sup> Ibero American Workshop on Nanostructures for Application in Micro and Optoelectronics*, November 2001, São José dos Campos, Brazil.
38. *Electric-field effects on the band-edge states of GaAs/AlAs coupled quantum wells*, F. J. Ribeiro, R. B. Capaz e B. Koiller, *phys. stat. sol. (b)* **232**, 148 (2002) - Proceedings of *Nano 2001: 2<sup>nd</sup> Ibero American Workshop on Nanostructures for Application in Micro and Optoelectronics*, November 2001, São José dos Campos, Brazil.
39. *Atomistic description of shallow levels in semiconductors*, A. S. Martins, J. G. Menchero, R. B. Capaz e B. Koiller, *Phys. Rev. B* **65**, 245205 (2002).
40. *Switching times in electric-field-tunable GaAs/AlAs heterostructures*, F. J. Ribeiro, R. B. Capaz e B. Koiller, *Appl. Phys. Lett.* **81**, 2247 (2002).
41. *Electromechanical effects in carbon nanotubes: Ab initio and analytical tight-binding calculations*, M. Verissimo-Alves, B. Koiller, H. Chacham, and R. B. Capaz, *Phys. Rev. B* **67**, 161401(R) (2003).
42. *Ab initio calculations of structural and dynamical properties of poly(p-phenylene) and poly(p-phenylene vinylene)*, R. B. Capaz e M. J. Caldas, *Phys. Rev. B* **67**, 205205 (2003).
43. *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 e R. B. Capaz, *Phys. Chem. Chem. Phys.* **5** (17), 3811-3817 (2003).
44. *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. Liu and M. Scheffler, *Phys. Rev. B* **68**, 235311 (2003).

45. *Electric-field control and adiabatic evolution of shallow donor impurities in silicon*, A. S. Martins, R. B. Capaz e B. Koiller, Phys. Rev. B **69**, 085320 (2004).
46. *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 e R. B. Capaz, Phys. Rev. B **70**, 085207 (2004).
47. *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 e S. Das Sarma, Phys. Rev. B **70**, 115207 (2004).
48. *Hydrostatic pressure effects on the structural and electronic properties of carbon nanotubes*, R. B. Capaz, C. D. Spataru, P. Tangney, M. L. Cohen e S. G. Louie, phys. stat. sol. (b) **241**, 3352 (2004) – Proceedings of The 11<sup>th</sup> International Conference on High Pressure Semiconductor Physics, 2-5 de agosto de 2004, Berkeley (CA), EUA.
49. *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).
50. *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).
51. *Theory of sodium ordering in  $\text{Na}_x\text{CoO}_2$* , P. H. Zhang, R. B. Capaz, M. L. Cohen, and S. G. Louie, Phys. Rev. B **71**, 153102 (2005).
52. *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).
53. *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).
54. *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).
55. *Application of standard DFT theory for nonbonded interactions in soft matter: Prototype study of poly-para-phenylene*, M. Alves-Santos, L. Y. A. Davila, H. M. Petrilli, R. B. Capaz, and M. J. Caldas, J. Comp. Chem. **27**, 217 (2006).
56. *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, M. Tinkham, Phys. Rev. Lett. **96**, 127403 (2006).
57. *Selection rules for one- and two-photon absorption by excitons in carbon nanotubes*, E. B. Barros, R. B. Capaz, A. Jorio, G. 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**, 241406(R) (2006).
58. *Review on the symmetry-related properties of carbon nanotubes*, E. B. Barros, A. Jorio, G. G. Samsonidze, R. B. Capaz, A. G. Souza Filho, J. Mendes, G. Dresselhaus, and M. S. Dresselhaus, Phys. Rep. **431**, 261 (2006).
59. *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).
60. *Straight to the bar: Molecular nanostructures, graphene, nanotubes*, R. B. Capaz, phys. stat. sol (RRL) **1**, A47 (2007).
61. *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 e B. Koiller, J. Appl. Phys. **102**, 023711 (2007).
62. *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).
63. *Chemical identification in the  $\text{Cu}_3\text{Au}(100)$  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).
64. *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).
65. *Early Stages of Vanadium Deposition on  $\text{Si}(111)-7\times 7$* , M. M. de Araújo, F. Stavale, A. A. Leitão, H. Niehus, C. A. Achete, and R. B. Capaz, Surf. Sci. **603**, 835 (2009).

66. *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. *Charge transfer and screening effects in polyynes encapsulated inside single-wall carbon nanotubes*, L. G. Moura, L. M. Malard, M. A. Carneiro, P. Venezuela, R. B. Capaz, D. Nishide, Y. Achiba, H. Shinohara, and M. A. Pimenta, *Phys. Rev. B* **80**, 161401(R) (2009).
68. *Experimental and theoretical investigation of tris-(8-hydroxy-quinolate) aluminum (Alq<sub>3</sub>) 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. *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. *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, R. B. Capaz, C.A. Achete, and A. Jorio, *Carbon* **48**, 1592 (2010).
71. *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. *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. *Signatures of oxygen on Cu<sub>3</sub>Au (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. *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. *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. *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. *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. *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. *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. *Hyperfine interactions in silicon quantum dots*, L. Assali, H. Petrilli, R. B. Capaz, B. Koiller, S. Das Sarma and X. Hu, *Phys. Rev. B*, *Phys. Rev. B* **83**, 165301 (2011).
81. *Heat pumping in nanomechanical systems*, C. Chamon, E. R. Mucciolo, L. Arrachea and R. B. Capaz, *Phys. Rev. Lett.* **106**, 135504 (2011).
82. *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. *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. *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. *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. *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. *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. *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. *First-principles calculations and XPS measurements of gold segregation at the Cu<sub>3</sub>Au(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. *Ab initio studies of pristine and oxidized Cu<sub>3</sub>Au(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. *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. *Microscopic model of a phononic refrigerator*, L. Arrachea, E. R. Mucciolo, C. Chamon, R. B. Capaz, Phys. Rev. B 86, 125424 (2012).
93. *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. *Structural determination of stable MoO<sub>x</sub> monolayers on O/Cu<sub>3</sub>Au(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. *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. *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. *First-principles studies of oxygen-induced copper segregation in Cu<sub>3</sub>Au(111)*, A. M. Silva, C. A. Achete and R. B. Capaz, Chem. Phys. 410, 99 (2013).
98. *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. *Molecular hyperfine fields in organic magnetoresistance devices*, R. Giro, F. P. Rosselli, R. S. Carvalho, R. B. Capaz, M. Cremona, C. A. Achete, Phys. Rev. B 87, 125204 (2013).
100. *Probing the electronic properties of ternary A<sub>n</sub>M<sub>3n-1</sub>B<sub>2n</sub> (n = 1: A = Ca, Sr; M = Rh, Ir and n=3: A = Ca, Sr; M = 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. *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. *A combined LEED and DFT surface structure determination of Cu<sub>3</sub>Au(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. *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. *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. *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. *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. *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. *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. *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. *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. *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. *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. *Effects of edge magnetism on the Kohn anomalies of zigzag graphene nanoribbons*, F. J. Culchac and R. B. Capaz, *Nanotechnology* 27, 065707 (2016).
114. *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. *Investigation of organic magnetoresistance dependence on spin-orbit coupling using  $\delta$ -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. *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. *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. Pénicau, C. A. Achete, R. B. Capaz and A. Jorio, *2D Mater.* 4, 025039 (2017).
118. *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. *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. *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. *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. *Van der Waals interactions and the properties of graphite and 2H-, 3R- and 1T-MoS<sub>2</sub>: A comparative study*, F. P. N. Antunes, V. S. Vaiss, S. R. Tavares, R. B. Capaz, A. A. Leitão, *Comp. Mat. Sci.* 152, 156 (2018).
123. *Electronic structure and optical properties of twisted multilayer graphene*, A. Vela, M. V. O. Moutinho, F. J. Culchac, P. Venezuela, and R. B. Capaz, *Phys. Rev. B* 98, 155135 (2018).
124. *Photonic spin Hall effect in bilayer graphene moiré superlattices*, W. J. M. Kort-Kamp, F. J. Culchac, R. B. Capaz, and F. A. Pinheiro, *Phys. Rev. B* 98, 195431 (2018).
125. *Theoretical characterization of hexagonal 2D  $\text{Be}_3\text{N}_2$  monolayer*, S. Ullah, P. A. Denis, R. B. Capaz, and F. Sato, *New J. Chem.* 43, 2933 (2019).
126. *Temperature effects on the structural phase transitions of gallium phosphide*, C.I. Ribeiro-Silva, A. Picinin, J.P. Rino, M. G. Menezes, R. B. Capaz, *Comp. Mater. Sci.* 161, 265 (2019).
127. *Novel 2D materials from exfoliation of layered hydroxide salts: A theoretical study*, S. R. Tavares, P. I. R. Moraes, R. B. Capaz, A. A. Leitão, *Appl. Surf. Sci.* 483, 762 (2019).
128. *Layer breathing and shear modes in multilayer graphene: a DFT-vdW study*, R. R. Del Grande, M. G. Menezes, R. B. Capaz, *J. Phys.: Condens. Matter* 31, 295301 (2019).
129. *Exotic impurity-induced states in single-layer h-BN: The role of sublattice structure and intervalley interactions*, S. Ullah, F. Sato, M. G. Menezes, R. B. Capaz, *Phys. Rev. B* 100, 085427 (2019).
130. *Spiro-Carbon: A Metallic Carbon Allotrope Predicted from First Principles Calculations*, F. L. Oliveira, R. B. Capaz, and P. M. Esteves, *ChemPhysChem* 21, 59 (2020).
131. *Energy barriers for collapsing large-diameter carbon nanotubes*, R.R. Del Grande, A. F. Fonseca, and R. B. Capaz, *Carbon* 159, 161 (2020).

132. *Flat bands and gaps in twisted double bilayer graphene*, F. J. Culchac, R. R. Del Grande, R. B. Capaz, L. Chico and E. Suárez Morell, *Nanoscale* 12, 5014 (2020).
133. *Graphene as interface modifier in ITO and ITO-Cr electrodes*, L. A. Silva, J. M. M. Luzardo, S. M. Oliveira, R. V. Curti, A. M. Silva, R. Valaski, R. B. Capaz, J. R. Araujo, *Curr. Appl. Phys.* 20, 846 (2020).
134. *Pressure dependence of room-temperature structural properties of  $\text{CaAl}_2\text{Si}_2$* , S. Strikos, B. Joseph, F. G. Alabarse, G. Valadares, D. G. Costa, Rodrigo B. Capaz and M. ElMassalami, *J. Phys.: Condens. Matter* 32, 365403 (2020).
135. *Structural and magnetic properties of a defective graphene buffer layer grown on  $\text{SiC}(0001)$ : a DFT study*, C. Pereyra Huelmo, M. G. Menezes, R. B. Capaz and P. A. Denis, *Phys. Chem. Chem. Phys.* 22, 16096 (2020).
136. *Electronic properties of substitutional impurities in graphene-like  $\text{C}_2\text{N}$ ,  $\text{tg-C}_3\text{N}_4$ , and  $\text{hg-C}_3\text{N}_4$* , S. Ullah, P. A. Denis, M. G. Menezes, F. Sato, and R. B. Capaz, *Phys. Rev. B* 102, 134112 (2020).
137. *Emission redshift in DCM2-doped  $\text{Alq}_3$  caused by nonlinear Stark shifts and Förster-mediated exciton diffusion*, G. Candiotto, R. Giro, B. A. C. Horta, F. P. Rosselli, M. de Cicco, C. A. Achete, M. Cremona, and R. B. Capaz, *Phys. Rev. B* 102, 235401 (2020).
138. *Theory of hole-spin qubits in strained germanium quantum dots*, L. A. Terrazos, E. Marcellina, Zhanning Wang, S. N. Coppersmith, Mark Friesen, A. R. Hamilton, Xuedong Hu, Belita Koiller, A. L. Saraiva, Dimitrie Culcer, and Rodrigo B. Capaz, *Phys. Rev. B* 103, 125201 (2021).
139. *Oxygen effects on the electronic transport in stanene*, F. W. N. Silva, E. B. Barros, and R. B. Capaz, *Nanotechnology* 32, 395201 (2021).
140. *Harnessing the photonic local density of states in graphene moiré superlattices*, W. J. M. Kort-Kamp, F. J. Culchac, F. S. S. Rosa, C. Farina, R. B. Capaz, and F. A. Pinheiro, *Phys. Rev. B* 103, 155423 (2021).
141. *Experimentos caseiros: Uma adaptação mão-na-massa da disciplina de Física Experimental II da UFRJ para o ensino remoto*, A. Hernández, A. Gomes, E. Sinnecker, R. Del Grande, R. Capaz, S. Cardoso, *Rev. Bras. de Ensino de Física* 43, e20210248 (2021).
142. *Franckeite as an Exfoliable Naturally Occurring Topological Insulator*, W. S. Paz, M. G. Menezes, N. N. Batista, G. Sanchez-Santolino, M. Velický, M. Varela, R. B. Capaz, and J. J. Palacios, *Nano Lett.* 21, 7781 (2021).
143. *Atomic-scale study of Si-doped AlAs by cross-sectional scanning tunneling microscopy and density functional theory*, D. Tjeertes, A. Vela, T. J. F. Verstijnen, E. G. Banfi, P. J. van Veldhoven, M. G. Menezes, R. B. Capaz, B. Koiller, and P. M. Koenraad, *Phys. Rev. B* 104, 125433 (2021).
144. *Reorganization Energy upon Controlled Intermolecular Charge-Transfer Reactions in Monolithically Integrated Nanodevices*, L. Merces, G. Candiotto, L. M. M. Ferro, A. de Barros, C. V. S. Batista, A. Nawaz, A. Riul Jr., R. B. Capaz, C. C. B. Bufon, *Small* 17, 2103897 (2021).
145. *Structural Metastability and Fermi Surface Topology of  $\text{SrAl}_2\text{Si}_2$* , S. Strikos, B. Joseph, F. G. Alabarse, G. Valadares, D. G. Costa, R. B. Capaz, and M. El Massalami, *Inorg. Chem.* 60, 18652 (2021).
146. *Spatially controlled graphene-MoSe<sub>2</sub> lateral heterostructure for sensing applications: Insights from first-principles calculations*, E. S. Souza, M. G. Menezes, W. L. Scopel, and R. B. Capaz, *Phys. Rev. B* 105, 115413 (2022).
147. *Stability and Rupture of an Ultrathin Ionic Wire*, B. Focassio, T. E. R. Fiuza, J. Bettini, G. R. Schleder, M. H. M. Rodrigues, J. B. Souza Junior, E. R. Leite, A. Fazzio, and Rodrigo B. Capaz, *Phys. Rev. Lett.* 129, 046101 (2022).
148. *Role of Functional Thiolated Molecules on the Enhanced Electronic Transport of Interconnected MoS<sub>2</sub> Nanostructures*, R. L. H. Freire, F. C. de Lima, R. F. de Oliveira, R. B. Capaz, A. Fazzio, *J. Phys. Chem. C* 126, 12159 (2022).
149. *Vibrational instabilities in multilayer graphene and graphite: Effects of strain and number of layers*, L. D. Zambrano Palma, M. G. Menezes, and R. B. Capaz, *Phys. Rev. B* 106, 195407 (2022).
150. *Grand Challenges in Graphene and Graphite Research*, R. B. Capaz, *Frontiers in Carbon* 1, 1034557 (2022).
151. *How lignin sticks to cellulose—insights from atomic force microscopy enhanced by machine-learning analysis and molecular dynamics simulations*, D. M. Nascimento, F. M. Colombari, B. Focassio, G. R. Schleder, C. A. R. Costa, C. A. Biffe, L. Y. Ling, R. F. Gouveia, M. Strauss, G. J. M. Rocha, E. Leite, A. Fazzio, R. B. Capaz, C. Driemeier and J. S. Bernardes, *Nanoscale* 14, 17561 (2022).



152. *Surface characterization using Friction Force Microscopy and the Jarzynski equality*, Y. Watanabe, R. B. Capaz, R. A. Simão, Appl. Surf. Sci. 607, 155070 (2023).
153. *FRET-Calculator: A free software and web server for Förster Resonance Energy Transfer Calculation*, L. Benatto, O. Mesquita, J. L. B. Rosa, L. S. Roman, M. Koehler, R. B. Capaz, and G. Candiotto, Computer Physics Communications 287, 108715 (2023).
154. *Resonance Raman spectroscopy characterization of linear carbon chains encapsulated by multi-walled carbon nanotubes*, T. A. Moura, W. Q. Neves, R. S. Alencar, Y.A. Kim, M. Endo, T. L. Vasconcelos, D. G. Costa, G. Candiotto, R. B. Capaz, P. T. Araujo, A. G. Souza Filho, A. R. Paschoal, Carbon 212, 118123 (2023).
155. *Improved Performance of Organic Light-Emitting Transistors Enabled by Polyurethane Gate Dielectric*, A. R. J. Barreto, G. Candiotto, H. J. C. Avila, R. S. Carvalho, A. M. dos Santos, M. Prosa, E. Benvenuti, S. Moschetto, S. Toffanin, R. B. Capaz, M. Muccini, and M. Cremona, ACS Appl. Mater. Interfaces 15, 33809 (2023).
156. *Patterning edge-like defects and tuning defective areas on the basal plane of ultra-large MoS<sub>2</sub> monolayers toward the hydrogen evolution reaction*, B. R. Florindo, L. H. Hasimoto, N. de Freitas, Graziani Candiotto, E. N. Lima, C. de Lourenço, A. B. S. de Araujo, C. Ospina, J. Bettini, E. R. Leite, R. S. Lima, A. Fazio, R. B. Capaz and M. Santhiago, J. Mater. Chem. A 11, 19890 (2023).
157. *CO adsorption on MgO thin-films: formation and interaction of surface charged defects*, R. S. Alvim, I. Borges Jr., R. M. B. Alves, R. B. Capaz and A. A. Leitão, Phys. Chem. Chem. Phys. 25, 28982 (2023).
158. *Unlocking the Potential of Nanoribbon-Based Sb<sub>2</sub>S<sub>3</sub>/Sb<sub>2</sub>Se<sub>3</sub> van-der-Waals Heterostructure for Solar-Energy-Conversion and Optoelectronics Applications*, V. G. Garcia, N. N. Batista, D. A. Aldave, R. B. Capaz, J. J. Palacios, M. G. Menezes, and W. S. Paz, ACS Appl. Mater. Interfaces 15, 54786 (2023).
159. *Enhancing the Chemical Stability and Photovoltaic Properties of Highly Efficient Nonfullerene Acceptors by Chalcogen Substitution: Insights from Quantum Chemical Calculations*, L. Benatto, J. P. A. Souza, M. F. F. das Neves, L. S. Roman, R. B. Capaz, G. Candiotto, and M. Koehler, ACS Appl. Energy Mater. 6, 11732 (2023).
160. *PLQ-sim: A computational tool for simulating photoluminescence quenching dynamics in organic donor/acceptor blends*, L. Benatto, O. Mesquita, L. S. Roman, R. B. Capaz, G. Candiotto, M. Koehler, Computer Physics Communications 296, 109015 (2024).
161. *Strain, anharmonicity, and finite-size effects on the vibrational properties of linear carbon chains*, G. Candiotto, F. R. Silva, D. G. Costa, and R. B. Capaz, Phys. Rev. B **109**, 045405 (2024).
162. *RI-Calculator: A user friendly software and web server for refractive index calculation*, L. Benatto, O. Mesquita, L.S. Roman, M. Koehler, R. B. Capaz, G. Candiotto, Computer Physics Communications 298, 109100 (2024).
163. *Visualization of electron beam-induced desintering of nanostructured ceramics at the atomic scale*, T. E. R. Fiuza, B. Focassio, J. Bettini, G. R. Schleder, M. H. M. Rodrigues, J. B. Souza Junior, A. Fazio, R. B. Capaz, and E. R. Leite, Cell Reports Physical Science 5, 101828 (2024).
164. *TMM-Sim: A versatile tool for optical simulation of thin-film solar cells*, L. Benatto, O. Mesquita, K. R. M. Pacheco, L. S. Roman, M. Koehler, R. B. Capaz, G. Candiotto, Computer Physics Communications 300, 109206 (2024).