Referências Bibliográficas

[AbsDaCruz, 2004] DA CRUZ, A. V. A.; PACHECO, M. A. C.; VELLASCO, M. B. R. ; BARBOSA, C. R. H.. **Cultural operators for a quantum-inspired evolutionary algorithm applied to numerical optimization problems**. In: IWINAC, volumen 2, Berlin, Germany, 2004. Springer-Verlag. 3.1.4, 3.1.4, 3.1.4

[AbsDaCruz, 2005] DA CRUZ, A. V. A.; BARBOSA, C. R. H.; PACHECO, M. A. C. ; VELLASCO, M. B. R.. **Quantum-inspired evolutionary algorithms and its application to numerical optimization problems**. In: ICONIP, Berlin, Germany, 2005. Springer-Verlag. 2.7

[Alexandrova, 2004] ALEXANDROVA, A.; BOLDYREV, A.; FU, Y.; YANG, X.; WANG, X. ; WANG, L.. **Structure of the NaCl (x= 1–4) clusters via ab initio genetic algorithm and photoelectron spectroscopy**. The Journal of Chemical Physics, 121:5709, 2004. 7.2, 7.2, 7.4.1

[Alexandrova, 2005] ALEXANDROVA, A.; BOLDYREV, A.. **Search for the Li n 0/(n) 5-7) Lowest-Energy Structures Using the ab Initio Gradient Embedded Genetic Algorithm (GEGA). Elucidation of the Chemical Bonding in the Lithium Clusters**. J. Chem. Theory Comput, 1(4):566–580, 2005. 7.2, 7.2, 7.4.1, 7.4.1

[Arkhipov, 2006] ARKHIPOV, A.; FREDDOLINO, P. ; SCHULTEN, K.. **Stability and Dynamics of Virus Capsids Described by Coarse-Grained Modeling**. Structure, 14(12):1767–1777, 2006. 2.3.1

[Back, 1996] BÄCK, T.. **Evolutionary algorithms in theory and practice**. Oxford University Press New York, 1996. 3.1.1

[Bandow, 2006] BANDOW, B.; HARTKE, B.. **Larger Water Clusters with Edges and Corners on Their Way to Ice:# 160 Structural Trends Elucidated with an Improved Parallel Evolutionary Algorithm**. Journal of Physical Chemistry A, 110(17):5809–5822, 2006. 7.5, 7.5.1

[Bazterra, 2004] BAZTERRA, V.; OŃA, O.; CAPUTO, M.; FERRARO, M.; FUENTEALBA, P. ; FACELLI, J.. **Modified genetic algorithms to model**

cluster structures in medium-size silicon clusters. Physical Review A, 69(5):53202, 2004. 7.2

[Bhushan, 2007] BHUSHAN, B.. **Springer handbook of nanotechnology**. Springer, Berlin, 2007. 2.1, 2.1, 2.3.2, 2.4

[Bimberg, 1999] BIMBERG, D.; GRUNDMANN, M. ; LEDENTSOV, N.. **Quantum Dot Heterostructures**. Wiley, 1999. 4.2

[Bishop, 1970] BISHOP, D.; SOMORJAI, R.. **Integral-Transform Gaussian Functions for Heliumlike Systems**. Journal of Mathematical Physics, 11:1150, 1970. 6.2

[Bland, 2002] BLAND, S.. **Future challenges for MOVPE–an industrial perspective**. Journal of Materials Science: Materials in Electronics, 13(11):679–682, 2002. 4.2.1

[Borgstrom, 2003] BORGSTROM, M.; PIRES, M.; BRYLLERT, T.; LANDI, S.; SEIFERT, W. ; SOUZA, P.. **InAs quantum dots grown on InAlGaAs lattice matched to InP.** Journal of Crystal Growth, 252(4):481–485, 2003. 4.2.1

[Bryantsev, 2009] BRYANTSEV, V.; DIALLO, M.; VAN DUIN, A. ; GODDARD III, W.. **Evaluation of B3LYP, X3LYP, and M06-Class Density Functionals for Predicting the Binding Energies of Neutral, Protonated, and Deprotonated Water Clusters**. Journal of Chemical Theory and Computation, 5:1016–1026, 2009. 7.5.1

[Bunge,1992] BUNGE, C.; BARRIENTOS, J.; BUNGE, A. ; COGORDAN, J.. **Hartree-Fock and Roothaan-Hartree-Fock energies for the ground states of He through Xe**. Physical Review A, 46(7):3691–3696, 1992. 6.6, 6.6

[Burnham, 2002] BURNHAM, C.; XANTHEAS, S.. **Development of transferable interaction models for water. IV. A flexible, all-atom polarizable potential (TTM2-F) based on geometry dependent charges derived from an ab initio monomer dipole moment surface**. The Journal of Chemical Physics, 116:5115, 2002. 7.5, 7.5.1

[Callister, 1993] CALLISTER, W.. **Materials science and engineering: an introduction**. John Wiley & Sons New York, 1993. 4.3

[Cao, 1999] CAO, Y.; PARKER, I.; YU, G.; ZHANG, C. ; HEEGER, A.. **Improved quantum efficiency for electroluminescence in semiconducting polymers**. Nature, 397:414–417, 1999. 5.1

[Chattopadhyayfs, 1981] CHATTOPADHYAYFS, P.; DREIZLERI, R. ; TRSICJ, M.. **Application of the generator coordinate method to one-and two-electron atoms in an electric field**. J. Phys. B: At. Mol. Phys, 14:3849–3855, 1981. 6.3

[Chang, 1996] CHANG, C.; SZE, S.. **ULSI technology**. McGraw-Hill New York, 1996. D

[Chan, 2002] CHAN, C.; WU, J.; LI, J. ; CHEUNG, Y.. **Polypropylene/calcium carbonate nanocomposites**. Polymer, 43(10):2981–2992, 2002. B

[Clementi, 1990] CLEMENTI, E.; CHAKRAVORTY, S.; CORONGIU, G. ; SONNAD, V.. **Independent Electron Models: Hartree-Fock for Many-Electron Atoms**. MOTE CC-90 Modern Techniques in Computational Chemistry (E. Clementi, Ed.), Escom, Leiden, p. 90–72199, 1990. 6.1

[Cohentannoudji, 1979] COHEN-TANNOUDJI, C.; DIU, B.; LALÖ, F. ; CRASEMANN, B.. **Quantum Mechanics**. American Journal of Physics, 47:662, 1979. 2.3.2

[Davis, 1991] DAVIS, L.; OTHERS. **Handbook of genetic algorithms**. Van nostrand reinhold New York, 1991. 3.1.1

[Deaven, 1995] DEAVEN, D.; HO, K.. **Molecular Geometry Optimization with a Genetic Algorithm**. Physical Review Letters, 75(2):288–291, 1995. 7.2, 7.2, 7.3, 7.3.3

[Dowling, 2004] DOWLING, A.; CLIFT, R.; GROBERT, N. ; OTHERS. **Nanoscience and Nanotechnologies: Opportunities and Uncertainties**. The Royal Society and the Royal Academy of Engineering, 29, 2004. 2.1

[Doye, 2004] DOYE, J.; LEARY, R.; LOCATELLI, M. ; SCHOEN, F.. **Global Optimization of Morse Clusters by Potential Energy Transformations**. Informs Journal on Computing, 16(4):371–379, 2004. 7.1, 7.2

[Fagerstrom, 2002] FAGERSTROM, J.; FAXEN, T.; MUNGER, P.; YNNERMAN, A.; DESPLAT, J.; DE ANGELIS, F.; MERCURI, F.; ROSI, M.; SGAMELLOTTI, A.; TARANTELLI, F. ; OTHERS. **High Performance Computing Development for the Next Decade, and its Implications for Molecular Modelling Applications**. The ENACTS project, http://www. enacts. org. 2.6

[Fanourgakis, 2006] FANOURGAKIS, G.; XANTHEAS, S.. **The flexible, polarizable, thole-type interaction potential for water (TTM2-F) revisited**. J. Phys. Chem. A, 110(11):4100–4106, 2006. 7.5, 7.5.1

[Fernandez, 2009] FERNANDEZ-LIMA, F.; VILELANETO, O.; PIMENTEL, A.; PONCIANO, C.; PACHECO, M.; NASCIMENTO, M. ; SILVEIRA, E.. **A Theoretical and Experimental Study of Positive and Neutral LiF Clusters Produced by Fast Ion Impact on a Polycrystalline LiF Target**. The Journal of Physical Chemistry A, 113(9):1813–1821, 2009. 1.3, 7.4.1, 7.4.1

[Fernandez, 2009b] FERNANDEZ-LIMA, F.; VILELANETO, O.; PIMENTEL, A.; PONCIANO, M.; NASCIMENTO, M. ; SILVEIRA, E.. **Theoretical and Experimental Study of Negative LiF Clusters Produced by Fast Ion Impact on a Polycrystalline $_7LiF$ Target**. The Journal of Physical Chemistry A, to appear, 2009. 7.4.3

[Fogel, 1966] FOGEL, L.. **Artificial intelligence through simulated evolution**. New York: John Wiley & Sons, 1966., 1966. 3.1.1

[Foresman, 1996] FORESMAN, J.; FRISCH, A.. **Exploring chemistry with electronic structure methods**. 1996. 2.3.1

[Fornes, 2003] FORNES, T.; PAUL, D.. **Modeling properties of nylon 6/clay nanocomposites using composite theories**. Polymer, 44(17):4993–5013, 2003. 4.3, 4.3.1

[Fu, 2006] FU, J.; NAGUIB, H.. **Effect of Nanoclay on the Mechanical Properties of PMMA/Clay Nanocomposite Foams**. Journal of Cellular Plastics, 42(4):325, 2006. B

[Fukui, 1991] FUKUI, T.; ANDO, S.; TOKURA, Y. ; TORIYAMA, T.. **GaAs tetrahedral quantum dot structures fabricated using selective area metalorganic chemical vapor deposition**. Applied Physics Letters, 58:2018, 1991. 4.2

[G03] FRISCH, M. J.; TRUCKS, G. W.; SCHLEGEL, H. B.; SCUSERIA, G. E.; ROBB, M. A.; CHEESEMAN, J. R.; MONTGOMERY, JR., J. A.; VREVEN, T.; KUDIN, K. N.; BURANT, J. C.; MILLAM, J. M.; IYENGAR, S. S.; TOMASI, J.; BARONE, V.; MENNUCCI, B.; COSSI, M.; SCALMANI, G.; REGA, N.; PETERSSON, G. A.; NAKATSUJI, H.; HADA, M.; EHARA, M.; TOYOTA, K.; FUKUDA, R.; HASEGAWA, J.; ISHIDA, M.; NAKAJIMA, T.; HONDA, Y.; KITAO, O.; NAKAI, H.; KLENE, M.; LI, X.; KNOX, J. E.; HRATCHIAN, H. P.; CROSS, J. B.; BAKKEN, V.; ADAMO, C.; JARAMILLO, J.; GOMPERTS, R.; STRATMANN, R. E.; YAZYEV, O.; AUSTIN, A. J.; CAMMI, R.; POMELLI, C.; OCHTERSKI, J. W.; AYALA, P. Y.; MOROKUMA, K.; VOTH, G. A.; SALVADOR, P.; DANNENBERG,

J. J.; ZAKRZEWSKI, V. G.; DAPPRICH, S.; DANIELS, A. D.; STRAIN, M. C.; FARKAS, O.; MALICK, D. K.; RABUCK, A. D.; RAGHAVACHARI, K.; FORESMAN, J. B.; ORTIZ, J. V.; CUI, Q.; BABOUL, A. G.; CLIFFORD, S.; CIOSLOWSKI, J.; STEFANOV, B. B.; LIU, G.; LIASHENKO, A.; PISKORZ, P.; KOMAROMI, I.; MARTIN, R. L.; FOX, D. J.; KEITH, T.; AL-LAHAM, M. A.; PENG, C. Y.; NANAYAKKARA, A.; CHALLACOMBE, M.; GILL, P. M. W.; JOHNSON, B.; CHEN, W.; WONG, M. W.; GONZALEZ, C. ; POPLE, J. A.. **Gaussian 03, Revision C.02**. Gaussian, Inc., Wallingford, CT, 2004. 6.5, 6.6, 7.4.1

[Gibson, 1994] GIBSON, R.. **Principles of composite material mechanics**. McGraw-Hill, New York, 1994. 4.3

[Goasguen, 2005] GOASGUEN, S.; MADHAVAN, K.; MCLENNAN, M.; LUNDSTORM, M. ; KLIMECK, G.. **The NanoHUB: A Science Gateway for the Computational Nanotechnology Community**. Workshop on Science Gateways: Common Community Interfaces to Grid Resources, GGF, 14, 2005. 2.5

[Gojny, 2004] GOJNY, F.; WICHMANN, M.; KÖPKE, U.; FIEDLER, B. ; SCHULTE, K.. **Carbon nanotube-reinforced epoxy-composites: enhanced stiffness and fracture toughness at low nanotube content**. Composites Science and Technology, 64(15):2363–2371, 2004. B

[Gojny, 2005] GOJNY, F.; WICHMANN, M.; FIEDLER, B. ; SCHULTE, K.. **Influence of different carbon nanotubes on the mechanical properties of epoxy matrix composites–A comparative study**. Composites Science and Technology, 65(15-16):2300–2313, 2005. B

[Goldberg, 1989] GOLDBERG, D.. **Genetic algorithms in search, optimization and machine learning**. Addison-Wesley Longman Publishing Co., Inc. Boston, MA, USA, 1989. 3.1.1

[Gomes, 2006] GOMES, A.; CUSTODIO, R.. **Polynomial expansion of basis sets: Alternatives to fully optimized exponents**. Journal of Molecular Structure: THEOCHEM, 760(1-3):39–44, 2006. 6.2, 6.4, 6.5, 6.6

[Goodman, 1998] GOODMAN, J.. **Chemical Applications of Molecular Modeling**. Royal Society of Chemistry, The, 2007. 2.3.4

[Greenham, 1993] GREENHAM, N.; MORATTI, S.; BRADLEY, D.; FRIEND, R. ; HOLMES, A.. **Efficient light-emitting diodes based on polymers with high electron affinities**. 1993. 5.1

[Griffin, 1957] GRIFFIN, J.. **Collective Motions in Nuclei by the Method of Generator Coordinates**. Physical Review, 108(2):311–327, 1957. 6.3

[Grundmann, 2002] GRUNDMANN, M.. **Nano-Optoelectronics: Concepts, Physics, and Devices**. Springer, 2002. 4.2

[Gu, 2006] GU, Y.; VANCOURT, T. ; HERBORDT, M.. **Accelerating molecular dynamics simulations with configurable circuits**. Computers and Digital Techniques, IEE Proceedings-, 153(3):189–195, 2006. 2.6

[Guimarães, 2002] GUIMARÃES, F.; BELCHIOR, J.; JOHNSTON, R. ; ROBERTS, C.. **Global optimization analysis of water clusters (HO)(11<n<13) through a genetic evolutionary approach**. The Journal of Chemical Physics, 116:8327, 2002. 7.5

[Gusso, 2004] GUSSO, A.; MA, D.; HÜMMELGEN, I. ; DA LUZ, M.. **Modeling of organic light-emitting diodes with graded concentration in the emissive multilayer**. Journal of Applied Physics, 95:2056, 2004. (document), 2.5, 5.1, 5.1.1, 5.1.2, 5.1.2, 5.1.3, 5.2, 5.1.3, 5.3, 5.1.3

[Haketa, 2002] HAKETA, N.; YOKOYAMA, K.; TANAKA, H. ; KUDO, H.. **Theoretical study on the geometric and electronic structure of the lithium-rich LinFn- 1 (n= 2–5) clusters**. Journal of Molecular Structure: THEOCHEM, 577(1):55–67, 2002. 7.4.1, 7.4.2

[Han, 2000] HAN, K.; KIM, J.. **Genetic quantum algorithm and its application to combinatorial optimization problem**. In: PROCEEDINGS OF THE 2000 CONGRESS ON EVOLUTIONARY COMPUTATION, volumen 2, p. 1354–1360, 2000. 2.7, 3.1.4, 3.1.4, 3.1.4

[Han, 2002] HAN, K.; KIM, J.. **Quantum-inspired evolutionary algorithm for a class of combinatorial optimization**. IEEE transactions on evolutionary computation, 6(6):580–593, 2002. 3.1.4, 3.1.4, 3.1.4

[Hartke, 1993] HARTKE, B.. **Global geometry optimization of clusters using genetic algorithms**. The Journal of Physical Chemistry, 97(39):9973–9976, 1993. 7.2

[Harima, 2000] HARIMA, Y.; KUNUGI, Y.; YAMASHITA, K. ; SHIOTANI, M.. **Determination of mobilities of charge carriers in electrochemically anion-doped polythiophene film**. Chemical Physics Letters, 317(3-5):310–314, 2000. 5.1.1

[Hartke, 2001] HARTKE, B.; FLAD, H. ; DOLG, M.. **Structures of mercury clusters in a quantum–empirical hybrid model**. Physical Chemistry Chemical Physics, 3(23):5121–5129, 2001. 7.2

[Hartke, 2003] HARTKE, B.. **Size-dependent transition from all-surface to interior-molecule structures in pure neutral water clusters**. Physical Chemistry Chemical Physics, 5(2):275–284, 2003. 7.2

[Haykin, 1999] HAYKIN, S.. **Neural Networks – A Comprehensive Foundation**. Prentice Hall, 2 edition, 1999. 3.2.3, 4.2.1

[Hill, 1953] HILL, D.. **Nuclear Constitution and the Interpretation of Fission Phenomena**. Physical Review, 89(5):1102–1145, 1953. 6.3

[Hohenberg, 1964] HOHENBERG, P.; KOHN, W.. **Inhomogeneous Electron Gas**. Physical Review, 136:B864, 1964. 2.3.2

[Hong, 2005] HONG, Z.; ZHANG, P.; HE, C.; QIU, X.; LIU, A.; CHEN, L.; CHEN, X. ; JING, X.. **Nano-composite of poly (l-lactide) and surface grafted hydroxyapatite: Mechanical properties and biocompatibility**. Biomaterials, 26(32):6296–6304, 2005. B

[Hopfield, 1982] HOPFIELD, J.. **Neural networks and physical systems with emergent collective computational abilities**. Proceedings of the national academy of sciences, 79(8):2554–2558, 1982. 3.2.1

[Hussain, 2007] HUSSAIN, F.; ROY, S.; NARASIMHAN, K.; VENGADASSALAM, K. ; LU, H.. **E-Glass Polypropylene Pultruded Nanocomposite: Manufacture, Characterization, Thermal and Mechanical Properties**. Journal of Thermoplastic Composite Materials, 20(4):411, 2007. B

[Jo, 2008] JO, B.; PARK, S. ; KIM, D.. **Mechanical properties of nano-MMT reinforced polymer composite and polymer concrete**. Construction and Building Materials, 22(1):14–20, 2008. B

[Johnson, 2002] JOHNSON, S.; JOANNOPOULOS, J.. **The MIT Photonic-Bands Package**. a href="http://ab-initio. mit. edu/mpb/» http://ab-initio. mit. edu/mpb/</a. 2.5

[Johnston, 2003] JOHNSTON, R.. **Evolving better nanoparticles: Genetic algorithms for optimising cluster geometries**. Dalton Transactions, 2003(22):4193–4207, 2003. 7.1, 7.2, 7.2, 7.3.3

[Jorge, 1997] JORGE, F.; DE CASTRO, E. ; DA SILVA, A.. **Accurate universal Gaussian basis set for hydrogen through lanthanum generated with the generator coordinate Hartree-Fock method**. Chemical Physics, 216(3):317–321, 1997. 6.3

[Jorge, 1999b] JORGE, F.; MUNIZ, E.. **Accurate adapted Gaussian basis sets for the atoms from H through Xe**. International Journal of Quantum Chemistry, 71(4):307–312, 1999. 6.3

[Jorge, 1999] JORGE, F.; DE CASTRO, E.. **Improved generator coordinate Hartree–Fock method: application to first-row atoms**. Chemical Physics Letters, 302(5-6):454–460, 1999. 6.3, 6.5, 6.6, 6.6, 6.6, 6.6

[Kadau, 2006] KADAU, K.; GERMANN, T. ; LOMDAHL, P.. **Molecular dynamics comes of age: 320 billion atom simulation on BlueGene/L**. Int. J. Mod. Phys. C, 17:1755–1761, 2006. 2.3.1

[Klobukowski, 1993] KLOBUKOWSKI, M.. **Comparison of generator formulas for exponential parameters of Gaussian basis sets**. Chemical Physics Letters, 214, 2:166–174, 1993. 6.4, 6.4

[Klobukowski, 1994] KLOBUKOWSKI, M.. **Systematic sequences of well-balanced Gaussian basis sets**. Canadian Journal of Chemistry, 72(7):1741–1752, 1994. (document), 6.4, 6.4, 6.6, 6.7, 6.8, 6.9, 6.6

[Koehler, 2000] KOEHLER, M.; DA LUZ, M. ; HUMMELGEN, I.. **Bipolar tunnelling injection into single-layer organic light emitting devices: analytical solution using the regional approximation**. Journal of Physics D: Applied Physics, 33(17):2096–2107, 2000. 5.1

[Kohn, 1965] KOHN, W.; SHAM, L.. **Self-Consistent Equations Including Exchange and Correlation Effects**. Physical Review, 1965. 2.3.2

[Koza, 1992] KOZA, J.. **Genetic programming: on the programming of computers by means of natural selection**. MIT press, 1992. 3.1.1

[Kulkarni, 2008] KULKARNI, A.; GADRE, S. ; NAGASE, S.. **Quantum chemical and electrostatic studies of anionic water clusters,(H2O) n**. Journal of Molecular Structure: THEOCHEM, 851(1-3):213–219, 2008. 7.5

[Lagutschenkov, 2005] LAGUTSCHENKOV, A.; FANOURGAKIS, G.; NIEDNER-SCHATTEBURG, G. ; XANTHEAS, S.. **The spectroscopic signature of the “all-surface” to “internally solvated” structural

transition in water clusters in the n= 17–21 size regime. The Journal of chemical physics, 122:194310, 2005. 7.5.1

[Lathouwers, 1978] LATHOUWERS, L.. **Generator-coordinate theory of molecular spectra**. Physical Review A, 18(5):2150–2158, 1978. 6.3

[Leach, 2001] LEACH, A.. **Molecular Modelling: Principles and Applications**. Prentice Hall, 2001. 2.3.2, 2.3.2, 2.3.2, 2.3.2, 2.3.2, 2.3.2, 2.3.4, 6.2

[Lent, 1994] LENT, C.; TOUGAW, P. ; POROD, W.. **Logical devices implemented using quantum cellular automata**. J. Appl. Phys, 75:1818–1825, 1994. 5.2, 5.2.1

[Likholyot, 2007] LIKHOLYOT, A.; LEMKE, K.; HOVEY, J. ; SEWARD, T.. **Mass spectrometric and quantum chemical determination of proton water clustering equilibria**. Geochimica et Cosmochimica Acta, 71(10):2436–2447, 2007. 7.5

[Ma, 2000] MA, D.; HÜMMELGEN, I.; JING, X.; HONG, Z.; WANG, L.; ZHAO, X.; WANG, F. ; KARASZ, F.. **Charge transport in a blue-emitting alternating block copolymer with a small spacer to conjugated segment length ratio**. Journal of Applied Physics, 87:312, 2000. 5.1

[Ma, 2002] MA, D.; LEE, C.; LEE, S. ; HUNG, L.. **Improved efficiency by a graded emissive region in organic light-emitting diodes**. Applied Physics Letters, 80:3641, 2002. (document), 5.1, 5.1.1, 5.1.3, 5.3, 5.1.3, 5.1.3

[Mackay, 1992] MACKAY, D.. **Bayesian interpolation**. Neural computation, 4(3):415–447, 1992. 3.2.3

[Malliaras, 1998] MALLIARAS, G.; SCOTT, J.. **The roles of injection and mobility in organic light emitting diodes**. Journal of Applied Physics, 83:5399, 1998. 5.1

[Mansoori, 2005] MANSOORI, G.. **Principles of Nanotechnology: Molecular-Based Study of Condensed Matter in Small Systems**. World Scientific, 2005. 2.1

[Michalewicz, 1994] MICHALEWICZ, Z.. **Genetic algorithms + data structures = evolution programs (2nd, extended ed.)**. Springer-Verlag New York, Inc., New York, NY, USA, 1994. 3.1.1, 3.1.2, 5.1.2, 5.1.2, 7.3.3

[Mitchell, 1996] MITCHELL, M.. **An introduction to genetic algorithms**. Bradford Books, 1996. 3.1.1

[Mohallem, 1986] MOHALLEM, J.; DREIZLER, R. ; TRSIC, M.. **A Griffin-Hill-Wheeler version of the Hartree-Fock equations**. International Journal of Quantum Chemistry, 30(s 20):45–55, 1986. 6.2, 6.3, 6.3

[Moore, 1995] MOORE, M.; NARAYANAN, A.. **Quantum-inspired computing**, 1995. 2.7

[Morgon, 2007] MORGON, N.; COUTINHO, K.. **Métodos de química teórica e modelagem molecular**. Livraria da Física, 2007. 2.3.2, 2.3.2

[Nguyen, 2008] NGUYEN, Q.; ONG, Y.; SOH, H. ; KUO, J.. **Multiscale Approach to Explore the Potential Energy Surface of Water Clusters (H2O) n < 8**. The Journal of Physical Chemistry A, 112(28):6257–6261, 2008. 7.5

[Pal, 2008] PAL, R.. **Mechanical properties of composites of randomly oriented platelets**. Composites Part A, 39(9):1496–1502, 2008. 4.3, 4.3.1, 4.3.1, 4.3.1, 4.3.1

[Partridge, 1989] PARTRIDGE, H.. **Near Hartree–Fock quality GTO basis sets for the first-and third-row atoms**. The Journal of Chemical Physics, 90:1043, 1989. 6.6, 6.6

[Pauling, 1985] PAULING, L.; WILSON, E.. **Introduction to Quantum Mechanics**. Dover Publications, 1985. 2.3.2

[Paul, 2006] PAUL, B.; FUJITA, S.; OKAJIMA, M. ; LEE, T.. **Modeling and analysis of circuit performance of ballistic CNFET**. Proceedings of the 43rd annual conference on Design automation, p. 717–722, 2006. 2.6

[Petroff, 1982] PETROFF, P.; GOSSARD, A.; LOGAN, R. ; WIEGMANN, W.. **Toward quantum well wires: Fabrication and optical properties**. Applied Physics Letters, 41:635, 1982. 4.2

[Poole, 2003] POOLE, C.; OWENS, F.. **Introduction to Nanotechnology**. Wiley-Interscience, 2003. 1.1

[Potter, 2000] POTTER, M.; JONG, K.. **Cooperative coevolution: An architecture for evolving coadapted subcomponents**. Evolutionary Computation, 8(1):1–29, 2000. 3.1.3

[Reed, 1986] REED, M.; BATE, R.; BRADSHAW, K.; DUNCAN, W.; FRENSLEY, W.; LEE, J. ; SHIH, H.. **Spatial quantization in GaAs–AlGaAs multiple quantum dots**. Journal of Vacuum Science & Technology B: Microelectronics and Nanometer Structures, 4:358, 1986. 4.2

[Reed, 1998] REED, R.; MARKS, R.. **Neural smithing: supervised learning in feedforward artificial neural networks**. MIT Press Cambridge, MA, USA, 1999. (document), 3.8, 3.2.3, 3.2.3, 3.2.3

[Ryzhii, 2004] RYZHII, V.; KHMYROVA, I.; RYZHII, M. ; MITIN, V.. **Comparison of dark current, responsivity and detectivity in different intersubband infrared photodetectors**. Semiconductor Science and Technology, 19(1):8–16, 2004. 4.2

[Schmidt, 2007] SCHMIDT, K.. **Nanofrontiers: Visions for the Future of Nanotechnology**. Washington, DC, Project on Emerging Nanotechnooogies. Retrieved from http://www. nanotech project. org/reports, 2007. 2.4, 4.1

[Scott, 1997] SCOTT, J.; KARG, S. ; CARTER, S.. **Bipolar charge and current distributions in organic light-emitting diodes**. Journal of Applied Physics, 82:1454, 1997. 5.1, 5.1.1

[Silva, 2006] DE ABREU E SILVA, E.; DUARTE, H. ; BELCHIOR, J.. **An approach based on genetic algorithms and DFT for studying clusters:(H2O) n (2 < n < 13) cluster analysis**. Chemical Physics, 323(2-3):553–562, 2006. 7.5

[Simpson, 1989] SIMPSON, J.; OTHERS. **Oxford English Dictionary**. Clarendon Oxford, 1989. 2.3

[Singulani, 2008] SINGULANI, A.; VILELA NETO, O.; AURÉLIO PACHECO, M.; VELLASCO, M.; PIRES, M. ; SOUZA, P.. **Computational intelligence applied to the growth of quantum dots**. Journal of Crystal Growth, 310(23):5063–5065, 2008. 1.3

[Somorjai, 1968] SOMORJAI, R.. **Integral Transform Functions. A New Class of Approximte Wave Funcrions**. 1968. 6.2

[Somorjai, 1969] SOMORJAI, R.. **Integral transform functions. A simple non-exponential orbital for the He series.** Chemical Physics Letters, 3(6):395–397, 1969. 6.2

[Souza, 2007] SOUZA, P. L.; LOPES, A. J.; GEBHARD, T.; UNTERRAINER, K.; PIRES, M. P.; VILLAS-BOAS, J. M.; VIEIRA, G. S.; GUIMARAES, P. S. S. ; STUDART, N.. **Quantum dot structures grown on al containing quaternary material for infrared photodetection beyond 10 mu m**. Applied Physics Letters, 90(17):173510, 2007. 4.2

[Spector, 2004] SPECTOR, L.. **Automatic Quantum Computer Programming – A Genetic Programming Approach**. Springer, 2004. 2.7

[Steiner, 2004] STEINER, T.. **Semiconductor Nanostructures for Optoelectronic Applications**. Artech House, 2004. 4.2, 4.2

[Szabo, 1989] SZABO, A.; OSTLUND, N.. **Modern quantum chemistry**. McGraw-Hill New York, 1989. 2.3.2, 6.1

[Tachibana, 2000] TACHIBANA, K.; SOMEYA, T.; ISHIDA, S. ; ARAKAWA, Y.. **Selective growth of InGaN quantum dot structures and their microphotoluminescence at room temperature**. Applied Physics Letters, 76:3212, 2000. 4.2

[Taniguchi, 1974] TANIGUCHI, N.; OTHERS. **On the Basic Concept of Nanotechnology**. Proc. Int. Conf. Prod. Eng, p. 18–23, 1974. 2.1

[Thio, 2002] THIO, Y.; ARGON, A.; COHEN, R. ; WEINBERG, M.. **Toughening of isotactic polypropylene with CaCO3 particles**. Polymer, 43(13):3661–3674, 2002. B

[Tjong, 2006] TJONG, S.. **Structural and mechanical properties of polymer nanocomposites**. Materials Science & Engineering R, 53(3-4):73–197, 2006. B

[Ufimtsev, 2008] UFIMTSEV, I.; MARTÍNEZ, T.. **Quantum Chemistry on Graphical Processing Units. 1. Strategies for Two-Electron Integral Evaluation**. J. Chem. Theory Comput, 4(2):222–231, 2008. 2.6

[Vianna, 2004] VIANNA, J.; CANUTO, S. ; FAZZIO, A.. **Teoria Quântica de Moléculas e Sólidos**. Editora Livraria de Física, 2004. 2.3.2

[VilelaNeto, 2006] NETO, O. P. V.. **Simulação e síntese automática de circuitos de autômatos celulares com pontos quânticos através de técnicas inteligentes**. Master's thesis, Pontifícia Universidade Católica do Rio de Janeiro, 2006. 5.2.1

[VilelaNeto, 2007] NETO, O.; PACHECO, M. ; BARBOSA, C.. **Neural Network Simulation and Evolutionary Synthesis of QCA Circuits**. IEEE TRANSACTIONS ON COMPUTERS, p. 191–201, 2007. (document), 2.6, 5.2, 5.2.2, 5.2.2, 5.9, 5.2.3, 5.10, 5.2.3

[Vostrikov, 2006] VOSTRIKOV, A.; DROZDOV, S.; RUDNEV, V. ; KURKINA, L.. **Molecular dynamics study of neutral and charged water clusters**. Computational Materials Science, 35(3):254–260, 2006. 7.5

[Walus, 2002] WALUS, K.; VETTETH, A.; JULLIEN, G. ; DIMITROV, V.. **Design AND Simulation OF Quantum-Dot Cellular Automata**. CMC Symp. on Microelectronics Research and Development in Canada, Ottawa, June, 2002. 2.5

[Walus, 2004] WALUS, K.; DYSART, T.; JULLIEN, G. ; BUDIMAN, R.. **QCADesigner: A rapid design and simulation tool for quantum-dot cellular automata**. IEEE Transactions on Nanotechnology, 3(1):26–31, 2004. 5.2.2

[Wang, 2004a] WANG, J.; PYRZ, R.. **Prediction of the overall moduli of layered silicate-reinforced nanocomposites–part I: basic theory and formulas**. Composites Science and Technology, 64(7-8):925–934, 2004. 4.3

[Wang, 2004b] WANG, J.; PYRZ, R.. **Prediction of the overall moduli of layered silicate-reinforced nanocomposites–part II: analyses**. Composites Science and Technology, 64(7-8):935–944, 2004. 4.3

[Wasserman, 1989] WASSERMAN, P.. **Neural computing: theory and practice**. Van Nostrand Reinhold Co. New York, NY, USA, 1989. 3.2.1, 3.2.1

[Webster, 2004] WEBSTER, T.; WAID, M.; MCKENZIE, J.; PRICE, R. ; EJIOFOR, J.. **Nano-biotechnology: carbon nanofibres as improved neural and orthopaedic implants**. Nanotechnology, 15(1):48–54, 2004. B

[Werner, 2003] WERNER, A.; LI, F.; HARADA, K.; PFEIFFER, M.; FRITZ, T. ; LEO, K.. **Pyronin B as a donor for n-type doping of organic thin films**. Applied Physics Letters, 82:4495, 2003. 5.1

[Wong, 1975] WONG, C.. **Generator-coordinate methods in nuclear physics**. Phys. Rep, 15(5), 1975. 6.3

[Wu, 2004] WU, Y.; JIA, Q.; YU, D. ; ZHANG, L.. **Modeling Youngś modulus of rubber–clay nanocomposites using composite theories**. Polymer Testing, 23(8):903–909, 2004. 4.3.1

[Xiao, 1993] XIAO, Y.; WILLIAMS, D.. **Genetic algorithm: a new approach to the prediction of the structure of molecular clusters**. Chemical Physics Letters, 215(1-3):17–24, 1993. 7.2

[Zebulum, 2002] ZEBULUM, R.; PACHECO, M. ; VELLASCO, M.. **Evolutionary Electronics: Automatic Design of Electronic Circuits and Systems by Genetic Algorithms**. CRC Press, 2002. 1.1

[Zeiri, 1995] ZEIRI, Y.. **Prediction of the lowest energy structure of clusters using a genetic algorithm**. Physical Review E, 51(4):2769–2772, 1995. 7.2

[Zeng, 2004] ZENG, J.; SALTYSIAK, B.; JOHNSON, W.; SCHIRALDI, D. ; KUMAR, S.. **Processing and properties of poly (methyl methacrylate)/carbon nano fiber composites**. Composites Part B, 35(2):173–178, 2004. B

[Zhang, 2004] ZHANG, Q.; YU, Z.; XIE, X. ; MAI, Y.. **Crystallization and impact energy of polypropylene/CaCO3 nanocomposites with nonionic modifier**. Polymer, 45(17):5985–5994, 2004. 4.3.1, 4.3.1, B

[Zurada, 1992] ZURADA, J.. **Introduction to artificial neural systems**. West Publishing Co. St. Paul, MN, USA, 1992. 3.2.3

A
Tabela com os Experimentos dos Pontos Quânticos

	Entradas						Saídas		
sample	fluxo de In	Esp. Base	Temp. Cresc.	T Cresc.	% In	% Al	Densidade	Altura	Desvio Padrão
	sccm	nm	°C	s			$10^8 PQ/cm^2$	nm	nm
1	60	50	500	3	100	0	13	15.5	1.7
2	60	50	500	3	100	0	1.5	12.4	1.9
3	60	50	500	3	100	0	2.4	17	1.1
4	60	50	500	3	100	0	1.8	13.8	1.5
5	72	50	500	2.4	100	0	0.76	11.9	1.2
6	60	50	500	3.6	100	0	4.76	13.7	1.5
7	60	50	490	3	100	0	1.88	11.7	1.1
8	60	50	500	4.2	100	0	8.5	15.1	0.8
9	60	50	500	4.8	100	0	3.16	12.6	1.1
10	60	50	500	4.6	100	0	3.32	16.2	1.1
11	60	50	500	3.9	100	0	5	15.4	0.8
12	60	50	540	4.2	100	0	64.75	26.5	3.8
13	60	50	520	4.2	100	0	78.25	18.7	2.8
14	60	50	540	4.2	100	0	23.56	29.2	5.9
15	60	50	515	4.2	100	0	50	18.5	1.5
16	66	50	520	4.2	100	0	66.5	17	2
17	30	50	520	4.2	100	0	0.48	25	1
18	76	50	520	4.2	100	0	52.25	13.8	2.8
19	60	50	520	4.2	100	0	92.75	16.1	2.9
20	60	50	520	3.8	100	0	74.5	22.5	3.7
21	60	50	520	3.2	100	0	18.5	26.6	2.1
22	60	500	500	5	52.9	0	105	7.42	1.71
23	60	500	500	5	49.1	0	39	10	1.5

	Entradas						Saídas		
sample	fluxo de In	Esp. Base	Temp. Cresc.	T Cresc.	% In	% Al	Densidade	Altura	Desvio Padrão
	sccm	nm	°C	s			$10^8 PQ/cm^2$	nm	nm
24	60	500	500	5	55.4	0	70.5	8.5	1.2
25	60	500	500	5	54.8	0	62	9.3	1.4
26	60	500	500	5	51.3	0	49	9.2	1.1
27	60	500	500	5	53.3	0	57.5	9.9	1.5
28	60	500	500	5.5	53	0	80	7.8	1.8
29	60	500	500	5.9	53.2	0	78.5	7.5	1.7
30	60	500	510	5.5	53	0	79	8	1.5
31	60	500	510	5.5	53	0	80	8.3	1.6
32	60	500	520	5.9	52.7	0	90	6	1
33	60	500	520	3.5	53.6	0	69	5.1	1
34	60	10	520	5.5	53.3	0	118	9.1	1.5
35	66	10	520	5.5	53.3	0	148	8.2	1.5
36	60	10	500	5.5	53.3	0	129	8.1	2
37	66	10	500	5.5	53.3	0	130	8.7	2.2
38	72	10	520	5.5	53.3	0	156	8.4	1.7
39	78	10	520	5.5	53.3	0	173	8.6	1.9
40	90	10	520	5.5	53.3	0	182	9	2.2
41	66	500	520	5.5	51.8	0	147	9.3	1.5
42	66	10	520	5.5	51.8	0	128	9.9	1
43	66	10	520	5.5	54.5	0	132	7.6	1.6
44	66	500	520	5.5	54.5	23.3	130	7.5	1.5
45	66	10	520	5.5	54.5	23	162	7.1	1.5
46	66	10	490	5.5	53.3	5.8	106.25	8.7	1.9
47	60	500	500	5	52.3	16.5	210	4.45	1.68

	Entradas						Saídas		
sample	fluxo de In	Esp. Base	Temp. Cresc.	T Cresc.	% In	% Al	Densidade	Altura	Desvio Padrão
	sccm	nm	°C	s			$10^8 PQ/cm^2$	nm	nm
48	60	500	500	5	50.2	29	91	6.85	2.02
49	60	500	500	5	52	16.5	87	5.95	3.18
50	60	500	500	5	53.4	16.5	138	5.5	1.97
51	60	500	500	5	52.6	11.2		6.16	2.11
52	60	500	500	5	53.4	14.5	67.5	7.7	1.7
53	60	500	500	5	53.4	19.3	75	8.6	1.8
54	66	500	520	5.5	52.8	19.3	89.5	7.49	1.64
55	66	500	520	5.5	50.3	19.3	109.0	7.76	1.69
56	66	500	520	5.5	52.5	19.3	100.0	7.66	1.59
57	66	1.5	520	5.5	52.5	19.3	120.0	9.15	2.1
58	66	500	520	5.5	52.5	19.3	83.0	8.57	1.81
59	66	1.5	500	5.5	52.5	19.3	54.3	4.09	1.39
60	66	1.5	500	6.3	52.5	19.3	235.3	7.83	2.25
61	66	1.5	500	5.9	52.5	16.5	192.0	7.86	2.47
62	66	1.5	520	5.5	52.5	16.1	108.25	3.57	0.94
63	66	500	520	5.5	53.7	16.1	138.8	8.93	1.99
64	66	500	520	6.3	52.6	16.1	126.5	6.57	1.49
65	69	1.5	500	6.3	52.3	18	111.75	11.7	1.18
66	66	500	520	6.3	52.3	0	114.8	8.53	1.61
67	66	500	520	6	52.3	29	113.0	9.06	4.03

B
Tabela com os Experimentos dos Nanocompósitos

Matrizes

– DGEBPA Diglicil éter de bisfenol A
– iPP Polipropileno isotático
– PA6 Poliamida 6 (nylon)
– PLLA Poli(L- Ácido Lático) (Poly-L-Lactide Acid)
– PMMA Polimetilmetacrilato
– PP Polipropileno
– PU Poliuretano
– UP Poliester não saturado (Unsaturated Polyester)

Cargas

– CB Carbono ativado (carbon black)
– CNF Nanofibra de carbono (carbon nanofiber)
– DWCNT Nanotubo de carbono de parede dupla (double wall carbon nanotube)
– MMT Montmorilonita
– MWCNT Nanotubo de carbono de paredes múltiplas (multiwall carbon nanotube)
– SWCNT Nanotubo de carbono de parede única (singlewall carbon nanotube)

Matriz	Carga	Concent. (wt%)	Tam. (nm)	Razão de Aspecto	E (GPA)	Referência
PU	–	–	–	–	0.004	(Webster, 2004)
PU	CNF	0.02	60	500	0.006	(Webster, 2004)
PU	CNF	0.1	60	500	0.022	(Webster, 2004)
PU	CNF	0.25	60	500	0.028	(Webster, 2004)
PP	–	–	–	–	0.71	(Zhang, 2004)
PP	$CaCO_3$	0.05	44	1	0.71	(Zhang, 2004)
PP	$CaCO_3$	0.1	44	1	0.74	(Zhang, 2004)
PP	$CaCO_3$	0.15	44	1	0.81	(Zhang, 2004)
PP	$CaCO_3$	0.15	44	1	0.78	(Zhang, 2004)
PP	$CaCO_3$	0.15	44	1	0.76	(Zhang, 2004)
PP	$CaCO_3$	0.15	44	1	0.74	(Zhang, 2004)
PP	$CaCO_3$	0.2	44	1	0.84	(Zhang, 2004)
iPP	–	–	–	–	1.437	(Thio, 2002)
iPP	$CaCO_3$	0.135068	160	1	1.691	(Thio, 2002)
iPP	$CaCO_3$	0.247934	160	1	1.871	(Thio, 2002)
iPP	$CaCO_3$	0.425868	160	1	1.973	(Thio, 2002)
iPP	$CaCO_3$	0.559779	220	1	2.697	(Thio, 2002)
iPP	$CaCO_3$	0.247934	370	1	1.682	(Thio, 2002)
iPP	$CaCO_3$	0.372974	370	1	1.785	(Thio, 2002)
iPP	$CaCO_3$	0.474052	370	1	2.44	(Thio, 2002)
iPP	$CaCO_3$	0.559779	560	1	2.867	(Thio, 2002)
PP	–	–	–	–	1.6	(Chan, 2002)
PP	$CaCO_3$	0.137352	44	1	2.7	(Chan, 2002)
PP	$CaCO_3$	0.137352	44	1	3	(Chan, 2002)
PP	$CaCO_3$	0.137352	44	1	2.5	(Chan, 2002)
PP	$CaCO_3$	0.242403	44	1	3	(Chan, 2002)
PP	$CaCO_3$	0.242403	44	1	2.6	(Chan, 2002)
PP	$CaCO_3$	0.242403	44	1	2.9	(Chan, 2002)
PP	$CaCO_3$	0.324431	44	1	2.6	(Chan, 2002)

Tabela B.1: Dados retirados de tabelas disponíveis na literatura.

Matriz	Carga	Concent. (wt%)	Tam. (nm)	Razão de Aspecto	E (GPa)	Referência
PMMA	–	–	–	–	4.7	(Zeng, 2004)
PMMA	CNF (PR21PS)	0.05	200	100	8	(Zeng, 2004)
PMMA	CNF (PR21PS)	0.1	200	100	7.7	(Zeng, 2004)
PMMA	CNF (PR24PS)	0.05	100	100	7.5	(Zeng, 2004)
PMMA	CNF (PR24PS)	0.1	100	100	7.6	(Zeng, 2004)
E–glass–PP	–	–	–	–	4.12	(Hussain, 2007)
E–glass–PP	MMT (1.28E)	0.01	1	200	6.68	(Hussain, 2007)
E–glass–PP	MMT (1.28E)	0.02	1	200	6.97	(Hussain, 2007)
E–glass–PP	MMT (1.28E)	0.03	1	200	7.1	(Hussain, 2007)
E–glass–PP	MMT (1.28E)	0.04	1	200	7.92	(Hussain, 2007)
E–glass–PP	MMT (1.28E)	0.05	1	200	8.23	(Hussain, 2007)
E–glass–PP	MMT (1.28E)	0.1	1	200	8.67	(Hussain, 2007)
PMMA	–	–	–	–	1.35	(Fu, 2006)
PMMA	MMT (20A)	0.005	2.42	200	1.72	(Fu, 2006)
PMMA	MMT (20A)	0.01	2.42	200	1.48	(Fu, 2006)
PMMA	MMT (20A)	0.02	2.42	200	1.39	(Fu, 2006)
PMMA	MMT (20A)	0.005	2.42	200	1.28	(Fu, 2006)
PMMA	MMT (20A)	0.01	2.42	200	1.26	(Fu, 2006)
PMMA	MMT (20A)	0.02	2.42	200	1.24	(Fu, 2006)
Epoxy	–	–	–	–	2.599	(Gojny, 2005)
Epoxy	CB	0.001	30	1	2.752	(Gojny, 2005)
Epoxy	CB	0.003	30	1	2.796	(Gojny, 2005)
Epoxy	CB	0.005	30	1	2.83	(Gojny, 2005)
Epoxy	SWCNT	0.0005	2	500	2.681	(Gojny, 2005)
Epoxy	SWCNT	0.001	2	500	2.691	(Gojny, 2005)
Epoxy	SWCNT	0.003	2	500	2.812	(Gojny, 2005)
Epoxy	DWCNT	0.001	2.8	500	2.785	(Gojny, 2005)
Epoxy	DWCNT	0.003	2.8	500	2.885	(Gojny, 2005)
Epoxy	DWCNT	0.005	2.8	500	2.79	(Gojny, 2005)
Epoxy	DWCNT–NH_2	0.001	2.8	500	2.61	(Gojny, 2005)
Epoxy	DWCNT–NH_2	0.003	2.8	500	2.944	(Gojny, 2005)
Epoxy	DWCNT–NH_2	0.005	2.8	500	2.978	(Gojny, 2005)
Epoxy	MWCNT	0.001	15	3333.3	2.78	(Gojny, 2005)
Epoxy	MWCNT	0.003	15	3333.3	2.765	(Gojny, 2005)
Epoxy	MWCNT	0.005	15	3333.3	2.609	(Gojny, 2005)
Epoxy	MWCNT–NH_2	0.001	15	3333.3	2.884	(Gojny, 2005)
Epoxy	MWCNT–NH_2	0.003	15	3333.3	2.819	(Gojny, 2005)
Epoxy	MWCNT–NH_2	0.005	15	3333.3	2.82	(Gojny, 2005)

Tabela B.2: Dados retirados de tabelas disponíveis na literatura. (continuação)

Matriz	Carga	Concent. (wt%)	Tam. (nm)	Razão de Aspecto	E (GPA)	Referência
Epoxy	–	–	–	–	3.282	(Gojny, 2004)
Epoxy	CB	0.1	30	1	3.297	(Gojny, 2004)
Epoxy	DWNT	0.1	2.8	2500	3.352	(Gojny, 2004)
Epoxy	DWNT–NH_2	0.1	2.8	2500	3.496	(Gojny, 2004)
Epoxy	DWNT–NH_2	1	2.8	2500	3.508	(Gojny, 2004)
UP	–	–	–	–	2.994631	(Jo, 2008)
UP	MMT Na+	0.02	1.17	100	3.087248	(Jo, 2008)
UP	MMT Na+	0.05	1.17	100	3.515436	(Jo, 2008)
UP	MMT Na+	0.08	1.17	100	3.230201	(Jo, 2008)
UP	MMT Na+	0.1	1.17	100	2.851678	(Jo, 2008)
UP	MMT (25A)	0.02	1.85	100	3.189262	(Jo, 2008)
UP	MMT (25A)	0.05	1.85	100	3.655034	(Jo, 2008)
UP	MMT (25A)	0.08	1.85	100	3.332886	(Jo, 2008)
UP	MMT (25A)	0.1	1.85	100	3.097315	(Jo, 2008)
UP	MMT (30B)	0.02	1.86	100	2.844295	(Jo, 2008)
UP	MMT (30B)	0.05	1.86	100	4.033557	(Jo, 2008)
UP	MMT (30B)	0.08	1.86	100	3.515436	(Jo, 2008)
UP	MMT (30B)	0.1	1.86	100	3.148322	(Jo, 2008)
PA6	–	–	–	–	20.17752	(Tjong, 2006)
PA6	SiO_2	0.05	12	1	22.37711	(Tjong, 2006)
PA6	SiO_2	0.1	12	1	24.19246	(Tjong, 2006)
PP	–	–	–	–	1.390909	(Tjong, 2006)
PP	SiO_2	0.01	12	1	1.421818	(Tjong, 2006)
PP	SiO_2	0.025	12	1	1.492727	(Tjong, 2006)
PP	SiO_2	0.05	12	1	1.565455	(Tjong, 2006)
PP	SiO_2	0.075	12	1	1.614545	(Tjong, 2006)
PP	SiO_2	0.1	12	1	1.690909	(Tjong, 2006)
PP	SiO_2	0.15	12	1	1.8	(Tjong, 2006)

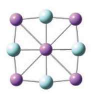
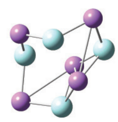
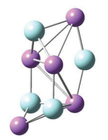
Tabela B.3: Dados retirados de gráficos disponíveis na literatura.

Matriz	Carga	Concent. (wt%)	Tam. (nm)	Razão de Aspecto	E (GPA)	Referência
PLLA (moulded)	–	–	–	–	1.855	(Hong, 2005)
PLLA (moulded)	g-HAP	0.02	20	5	2.34	(Hong, 2005)
PLLA (moulded)	g-HAP	0.04	20	5	2.553	(Hong, 2005)
PLLA (moulded)	g-HAP	0.06	20	5	2.553	(Hong, 2005)
PLLA (moulded)	g-HAP	0.08	20	5	2.644	(Hong, 2005)
PLLA (moulded)	g-HAP	0.1	20	5	2.68	(Hong, 2005)
PLLA (moulded)	g-HAP	0.15	20	5	2.98	(Hong, 2005)
PLLA (moulded)	g-HAP	0.2	20	5	3.161	(Hong, 2005)
PLLA (moulded)	HAP	0.02	20	5	2.34	(Hong, 2005)
PLLA (moulded)	HAP	0.04	20	5	2.42	(Hong, 2005)
PLLA (moulded)	HAP	0.06	20	5	2.526	(Hong, 2005)
PLLA (moulded)	HAP	0.08	20	5	2.631	(Hong, 2005)
PLLA (moulded)	HAP	0.1	20	5	2.651	(Hong, 2005)
PLLA (moulded)	HAP	0.15	20	5	2.954	(Hong, 2005)
PLLA (moulded)	HAP	0.2	20	5	3.051	(Hong, 2005)
PLLA (annealed)	–	–	–	–	3.064	(Hong, 2005)
PLLA (annealed)	HAP	0.02	20	5	3.257	(Hong, 2005)
PLLA (annealed)	HAP	0.04	20	5	3.201	(Hong, 2005)
PLLA (annealed)	HAP	0.06	20	5	3.311	(Hong, 2005)
PLLA (annealed)	HAP	0.08	20	5	3.533	(Hong, 2005)
PLLA (annealed)	HAP	0.1	20	5	3.617	(Hong, 2005)
PLLA (annealed)	HAP	0.15	20	5	3.641	(Hong, 2005)
PLLA (annealed)	HAP	0.2	20	5	3.851	(Hong, 2005)
PLLA (annealed)	g-HAP	0.02	20	5	3.233	(Hong, 2005)
PLLA (annealed)	g-HAP	0.04	20	5	3.286	(Hong, 2005)
PLLA (annealed)	g-HAP	0.06	20	5	3.365	(Hong, 2005)
PLLA (annealed)	g-HAP	0.08	20	5	3.557	(Hong, 2005)
PLLA (annealed)	g-HAP	0.1	20	5	3.514	(Hong, 2005)
PLLA (annealed)	g-HAP	0.15	20	5	3.832	(Hong, 2005)
PLLA (annealed)	g-HAP	0.2	20	5	3.988	(Hong, 2005)

Tabela B.4: Dados retirados de gráficos disponíveis na literatura. (continuação)

C
Resultados para os agregados de Li e F

Agregados de $(LiF)_4Li^+$

-437.5591057	-437.5363501	-437.5305583
		
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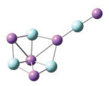	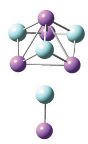	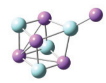
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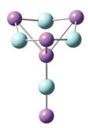	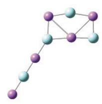	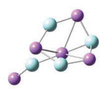
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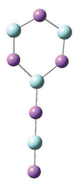	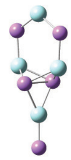	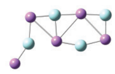
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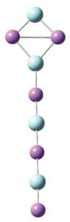	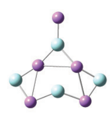	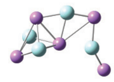
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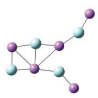
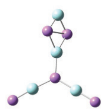
		

Tabela C.1: Estruturas dos aglomerados $(LiF)_4Li^+$.

Agregados de $(LiF)_4$

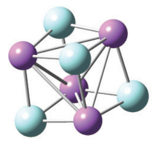
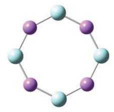
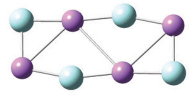
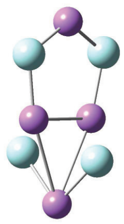
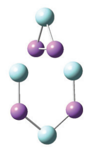
-430.1630023	-430.1497364	-430.1442856
		
-430.1251002	-430.1237355	
		

Tabela C.2: Estruturas dos aglomerados $(LiF)_4$.

Agregados de $(LiF)_4F^-$

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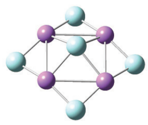
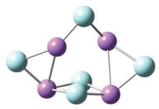
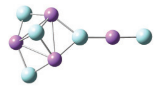
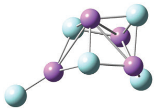
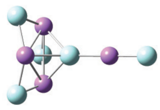
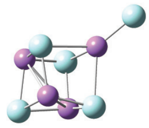
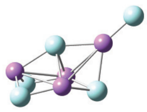
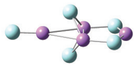
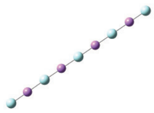
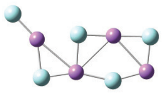
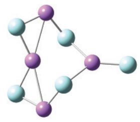
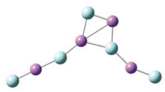
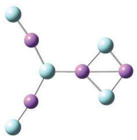
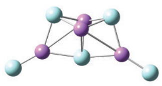
		
-530,114973	-530,113500	-530,112855
		
-530,111754	-530,109168	-530,107444
		
-530,106252	-530,096268	-530,093002
		
-530,086193	-530,082332	
		

Tabela C.3: Estruturas dos aglomerados $(LiF)_4F^-$.

Agregados de $(LiF)_5F^-$

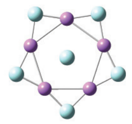
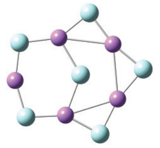
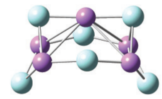
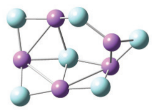
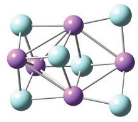
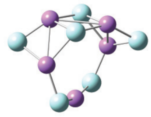
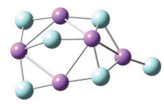
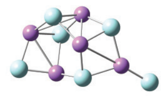
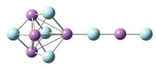
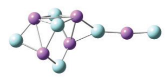
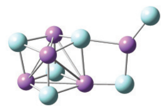
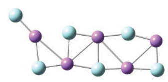
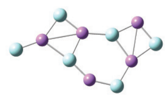
-637,703005	-637,702522	-637689894
		
-637,686801	-637,686789	-637,686729
		
-637,681344	-637,673634	-637,670310
		
-637,668581	-637,666413	-637,665640
		
-637,655340	-637,653673	
		

Tabela C.4: Estruturas dos aglomerados $(LiF)_5F^-$.

D
Síntese de OLEDs multicamadas

Dois M-OLEDs foram fabricados para verificar a validade experimental dos resultados encontrados nas simulações. O Alq_3 e o NPB foram usados tal como fornecidos para fabricar os dispositivos OLEDs. Anodos pré-padronizados de óxido de índio estanho (ITO) pré-depositados em substratos de vidro (com uma resistência de 8 (Ω/quadrado) foram limpos por tratamento RCA(Chang, 1996), enxaguados com água deionizada, seguido de sonicação em etanol por 10 minutos.

Depois da limpeza os substratos foram secados debaixo de nitrogênio. Camadas orgânicas foram depositadas em substratos à temperatura ambiente por evaporação térmica de cadinhos de quartzo resistivamente aquecidos em sistema com ambiente de alto vácuo, com uma pressão base em torno de $3.10^{-8} torr$ ($4.10^{-6} Pa$)

Os M-OLEDs foram montados usando-se uma heterojunção contendo uma camada de puro NPB (30nm), uma região graduada com cinco camadas internas co-depositada $NPB : Alq_3$ (10 nm de espessura cada) e uma pura camada de Alq_3 (20nm). A região graduada foi produzida por co-deposição de puro NPB e Alq_3 de duas fontes separadas. Finalmente, sem quebrar o vácuo, uma camada de 50nm de espessura de Mg:Ag (10:1) com uma camada protetora de prata (50nm), usada como catodo, foi co-evaporada a partir de cadinhos em taxa de 0.5nm/s em uma segunda câmara de vácuo. A espessura das camadas puras e a razão de NPB para Alq_3 em cada camada interna foi precisamente controlada por software in situ através de um monitor de cristal de quartzo. Os dispositivos eletroluminecentes fabricados apresentaram área ativa em torno de $3mm^2$ foram operadas em voltagens, com ITO como eletrodo positivo e $Mg : Ag/Ag$ como eletrodo negativo. Os dispositivos foram transferidos diretamente do sistema de deposição para uma câmara manipuladora com atmosfera controlada de N_2 e caracterizada dentro de uma hora após fabricação. O comportamento IxV e as medidas de brilho foram executadas usando-se um Keithlhey2400 calibrado e um Radiômetro/Fotômetro fabricado por United Detector Technology (UDT-350).

E
Publicações

Publicados

1. Fernandez-Lima, F. A. ; VILELA NETO, Omar Paranaiba ; Pimentel, A. S. ; Ponciano, C. R. ; Pacheco, M. A. C. ; Nascimento, M. A. Chaer ; Silveira, E. F. da . A Theoretical and Experimental Study of Positive and Neutral LiF Clusters Produced by Fast Ion Impact on a Polycrystalline LiF Target. Journal of Physical Chemistry. A, Molecules, Spectroscopy, Kinetics, Environment, and General Theory, v. 113, p. 1813-1821, 2009.

2. Alberto Fernandez-Lima, Francisco ; Vilela Neto, Omar P. ; Silva Pimentel, André ; Pacheco, M. A. C. ; Ponciano, Cássia Ribeiro ; Nascimento, Marco Antonio Chaer ; da Silveira, E. F. . Theoretical and Experimental Study of Negative LiF Clusters Produced by Fast Ion Impact on a Polycrystalline LiF Target. The Journal of Physical Chemistry. A, v. 113, p. 15031-15040, 2009.

3. Quirino, W.G. ; Teixeira, K.C. ; LEGNANI, C. ; Calil, V.L. ; Messer, B. ; Neto, O.P. Vilela ; Pacheco, M.A.C. ; CREMONA, M. Improved multilayer OLED architecture using evolutionary genetic algorithm. Thin Solid Films, v. 518, p. 1382-1385, 2009.

4. Singulani, Anderson Pires ; VILELA NETO, Omar Paranaiba ; PACHECO, Marco Aurélio C ; Vellasco, Marley M. ; Pires, M. ; SOUZA, P. L. . COMPUTATIONAL INTELLIGENCE APPLIED TO THE GROWTH OF QUANTUM DOTS. Journal of Crystal Growth, v. 310, p. 5063-5065, 2008.

5. Sá, Leonardo Bruno de ; VILELA NETO, Omar Paranaiba ; Mesquita, Antônio ; PACHECO, Marco Aurélio C . Modelagem para simulação no SPICE de transistores de nanotubos de carbono. Revista Militar de Ciência e Tecnologia, v. XXV, p. 29-39, 2008.

6. VILELA NETO, Omar Paranaiba ; PACHECO, Marco Aurélio C ; BARBOSA, C. R. H. . Neural Network Simulation and Evolutionary Synthesis of QCA Circuits. IEEE Transactions on Computers, v. 56, p. 191-201, 2007.

Submetidos

1. SINGULANI, Anderson Pires; VILELA NETO, Omar Paranaiba ; PACHECO, Marco Aurélio C. Evolutionary Synthesis of Robust QCA Circuits. IEEE Transactions on Nanotechnology.

2. Cupertino, L.F. ; Vilela Neto, O.P. ; Pacheco, M.A.C. ; Vellasco, M.B.R. ; d'Almeida, J.R.M; Modeling Young's Modulus of Nanocomposites: A Neural Network Approach.

Em produção

1. Agregados de H_2O

2. 2 artigos sobre Funções de Bases