Ewerton Caetano

List of Publications by Year
in descending order

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111 papers	2,062 citations	236925 25 h-index	315739 38 g-index
113 all docs	113 docs citations	113 times ranked	2108 citing authors

#	Article	IF	Citations
1	Optical absorption measurements and optoelectronic DFT calculations for ethanol solvated quercetin and anhydrous/hydrated quercetin crystals. Journal of Solid State Chemistry, 2022, 312, 123242.	2.9	3
2	Vibrational spectroscopy and phononâ€related properties of monoclinic GABA, a nonâ€proteinogenic inhibitory neurotransmitter amino acid. Journal of Raman Spectroscopy, 2021, 52, 1294-1307.	2.5	1
3	mTORâ€“mLST8 interaction: hot spot identification through quantum biochemistry calculations. New Journal of Chemistry, 2020, 44, 20982-20992.	2.8	5
4	Novel Si-C compounds with semiconducting and metallic properties: A DFT study. Computational Materials Science, 2020, 183, 109800.	3.0	4
5	The urokinase plasminogen activator binding to its receptor: a quantum biochemistry description within an in/homogeneous dielectric function framework with application to uPAâ€“uPAR peptide inhibitors. Physical Chemistry Chemical Physics, 2020, 22, 3570-3583.	2.8	19
6	Thermal stability and electronic properties of boron nitride nanoflakes. Journal of Molecular Modeling, 2020, 26, 100.	1.8	6
7	Structural and Optoelectronic Properties of the Î±-, Î²-, and Î³-Glycine Polymorphs and the Glycine Dihydrate Crystal: A DFT Study. Crystal Growth and Design, 2019, 19, 5204-5217.	3.0	13
8	Structural, electronic, and optical properties of inhomogeneous Ca1âˆ'x Mg x O alloys. Journal of Applied Physics, 2019, 125, 155102.	2.5	5
9	Solid state properties of hydroxyurea: Optical absorption measurement and DFT calculations. Journal of Applied Physics, 2019, 125, 134901.	2.5	4
10	Rose Bengal incorporated to Î±-cyclodextrin microparticles for photodynamic therapy against the cariogenic microorganism Streptococcus mutans. Photodiagnosis and Photodynamic Therapy, 2019, 25, 111-118.	2.6	14
11	Vibrational Properties of Bulk Boric Acid2Aand3TPolymorphs and Their Two-Dimensional Layers: Measurements and Density Functional Theory Calculations. Journal of Physical Chemistry A, 2018, 122, 1312-1325.	2.5	10
12	Polarized Raman, <scp>FTIR,</scp> and <scp>DFT</scp> study of <scp>Na₂Ti₃O₇</scp> microcrystals. Journal of Raman Spectroscopy, 2018, 49, 538-548.	2.5	54
13	Computational investigation of the Î±₂Î²₁integrinâ€“collagen triple helix complex interaction. New Journal of Chemistry, 2018, 42, 17115-17125.	2.8	16
14	Vibrational Modes and Phonon and Thermodynamic Properties of the Metaboric Acid Polymorphs Î±-, Î²-, and Î³-(BOH)₃O₃ within a Density Functional Theory Framework. Journal of Physical Chemistry A, 2018, 122, 7628-7645.	2.5	4
15	Anhydrous proline crystals: Structural optimization, optoelectronic properties, effective masses and Frenkel exciton energy. Journal of Physics and Chemistry of Solids, 2018, 121, 36-48.	4.0	17
16	First-generation antipsychotic haloperidol: optical absorption measurement and structural, electronic, and optical properties of its anhydrous monoclinic crystal by first-principle approaches. New Journal of Chemistry, 2018, 42, 13629-13640.	2.8	9
17	Quantum binding energy features of the T3-785 collagen-like triple-helical peptide. RSC Advances, 2017, 7, 2817-2828.	3.6	25
18	The vibrational properties of the bee-killer imidacloprid insecticide: A molecular description. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2017, 185, 245-255.	3.9	20

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19	An improved quantum biochemistry description of the glutamateâ€“GluA2 receptor binding within an inhomogeneous dielectric function framework. New Journal of Chemistry, 2017, 41, 6167-6179.	2.8	8
20	Structural, electronic and optical properties of monoclinic Na 2 Ti 3 O 7 from density functional theory calculations: A comparison with XRD and optical absorption measurements. Journal of Solid State Chemistry, 2017, 250, 68-74.	2.9	38
21	Energetic description of cilengitide bound to integrin. New Journal of Chemistry, 2017, 41, 11405-11412.	2.8	20
22	Improved description of the structural and optoelectronic properties of DNA/RNA nucleobase anhydrous crystals: Experiment and dispersion-corrected density functional theory calculations. Physical Review B, 2017, 96, .	3.2	13
23	Encapsulation of nor-Î²-lapachone into poly(<scp>d</scp>,<scp>l</scp>)-lactide-co-glycolide (PLGA) microcapsules: full characterization, computational details and cytotoxic activity against human cancer cell lines. MedChemComm, 2017, 8, 1993-2002.	3.4	6
24	Changing the gap type of solid state boric acid by heating: a dispersion-corrected density functional study of Î±-, Î²-, and Î³-metaboric acid polymorphs. New Journal of Chemistry, 2017, 41, 15533-15544.	2.8	4
25	Controlled Release of Nor-Î²-lapachone by PLGA Microparticles: A Strategy for Improving Cytotoxicity against Prostate Cancer Cells. Molecules, 2016, 21, 873.	3.8	17
26	A quantum biochemistry model of the interaction between the estrogen receptor and the two antagonists used in breast cancer treatment. Computational and Theoretical Chemistry, 2016, 1089, 21-27.	2.5	25
27	Structural, Electronic, and Optical Properties of Bulk Boric Acid 2A and 3T Polymorphs: Experiment and Density Functional Theory Calculations. Crystal Growth and Design, 2016, 16, 6631-6640.	3.0	13
28	Two Binding Geometries for Risperidone in Dopamine D3 Receptors: Insights on the Fast-Off Mechanism through Docking, Quantum Biochemistry, and Molecular Dynamics Simulations. ACS Chemical Neuroscience, 2016, 7, 1331-1347.	3.5	14
29	DFT Calculations with van der Waals Interactions of Hydrated Calcium Carbonate Crystals CaCO₃Â·(H₂O, 6H₂O): Structural, Electronic, Optical, and Vibrational Properties. Journal of Physical Chemistry A, 2016, 120, 5752-5765.	2.5	31
30	Computational electronic structure of the bee killer insecticide imidacloprid. New Journal of Chemistry, 2016, 40, 10353-10362.	2.8	12
31	A quantum chemistry investigation of a potential inhibitory drug against the dengue virus. RSC Advances, 2016, 6, 56562-56570.	3.6	28
32	Elucidating the high-k insulator Î±-Al2O3 direct/indirect energy band gap type through density functional theory computations. Chemical Physics Letters, 2015, 637, 172-176.	2.6	40
33	Electronic transport in methylated fragments of DNA. Applied Physics Letters, 2015, 107, 203701.	3.3	9
34	Quantum molecular modelling of ibuprofen bound to human serum albumin. RSC Advances, 2015, 5, 49439-49450.	3.6	42
35	Vibrational Spectroscopy and Phonon-Related Properties of the <scp>l</scp>-Aspartic Acid Anhydrous Monoclinic Crystal. Journal of Physical Chemistry A, 2015, 119, 11791-11803.	2.5	22
36	A quantum biochemistry investigation of willardiine partial agonism in AMPA receptors. Physical Chemistry Chemical Physics, 2015, 17, 13092-13103.	2.8	31

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37	Optical Absorption of the Antitrypanocidal Drug Benznidazole inWater. Molecules, 2014, 19, 4145-4156.	3.8	10
38	Conductance of single microRNAs chains related to the autism spectrum disorder. Europhysics Letters, 2014, 107, 68006.	2.0	11
39	L-asparagine crystals with wide gap semiconductor features: Optical absorption measurements and density functional theory computations. Journal of Chemical Physics, 2014, 140, 124511.	3.0	15
40	Phosphate group vibrational signatures of the osteoporosis drug alendronate. Journal of Raman Spectroscopy, 2014, 45, 801-806.	2.5	14
41	DNA-based nanobiostructured devices: The role of quasiperiodicity and correlation effects. Physics Reports, 2014, 535, 139-209.	25.6	88
42	Carbon-based nanorings sliding along inner coaxial nanotubes: MÃ¶bius topology effects in damping gigahertz oscillations. Journal of Applied Physics, 2014, 116, 124311.	2.5	4
43	Antipsychotic Haloperidol Binding to the Human Dopamine D3 Receptor: Beyond Docking Through QM/MM Refinement Toward the Design of Improved Schizophrenia Medicines. ACS Chemical Neuroscience, 2014, 5, 1041-1054.	3.5	37
44	A comparative density functional theory study of electronic structure and optical properties of -aminobutyric acid and its cocrystals with oxalic and benzoic acid. Chemical Physics Letters, 2013, 587, 20-24.	2.6	17
45	Assessing the Role of Water on the Electronic Structure and Vibrational Spectra of Monohydrated <scp>l</scp>-Aspartic Acid Crystals. Crystal Growth and Design, 2013, 13, 4844-4851.	3.0	22
46	An ab initio explanation of the activation and antagonism strength of an AMPA-sensitive glutamate receptor. RSC Advances, 2013, 3, 14988.	3.6	12
47	Quantum biochemistry study of the T3-785 tropocollagen triple-helical structure. Chemical Physics Letters, 2013, 559, 88-93.	2.6	31
48	<scp>l</scp>-Serine Anhydrous Crystals: Structural, Electronic, and Optical Properties by First-Principles Calculations, and Optical Absorption Measurement. Crystal Growth and Design, 2013, 13, 2793-2802.	3.0	27
49	Structural and optoelectronic properties, and infrared spectrum of cubic BaSnO3 from first principles calculations. Journal of Applied Physics, 2012, 112, .	2.5	54
50	Four-level levodopa adsorption on C60 fullerene for transdermal and oral administration: a computational study. RSC Advances, 2012, 2, 8306.	3.6	13
51	Inactivation of Ovine Cyclooxygenase-1 by Bromoaspirin and Aspirin: A Quantum Chemistry Description. Journal of Physical Chemistry B, 2012, 116, 3270-3279.	2.6	20
52	The DNA electronic specific heat at low temperature: The role of aperiodicity. Physics Letters, Section A: General, Atomic and Solid State Physics, 2012, 376, 2413-2417.	2.1	13
53	Electronic specific heat of an Î±3-helical polypeptide and its biochemical variants. Chemical Physics Letters, 2012, 542, 123-127.	2.6	3
54	Explaining statin inhibition effectiveness of HMG-CoA reductase by quantum biochemistry computations. Physical Chemistry Chemical Physics, 2012, 14, 1389-1398.	2.8	61

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55	Optical absorption and DFT calculations in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>L</mml:mi></mml:math>-aspartic acid anhydrous crystals: Charge carrier effective masses point to semiconducting behavior. Physical Review B, 2012, 86, .	3.2	51
56	Structural and electronic properties of SrxBa1â^'xSnO3 from first principles calculations. Journal of Solid State Chemistry, 2012, 187, 186-194.	2.9	47
57	Anhydrous crystals of DNA bases are wide gap semiconductors. Journal of Chemical Physics, 2011, 134, 175101.	3.0	45
58	Two-Level Adsorption of Ibuprofen on C₆₀ Fullerene for Transdermal Delivery: Classical Molecular Dynamics and Density Functional Theory Computations. Journal of Physical Chemistry C, 2011, 115, 24501-24511.	3.1	24
59	A renormalization approach to describe charge transport in quasiperiodic dangling backbone ladder (DBL)-DNA molecules. Physics Letters, Section A: General, Atomic and Solid State Physics, 2011, 375, 3993-3996.	2.1	14
60	Monoclinic and orthorhombic cysteine crystals are small gap insulators. Chemical Physics Letters, 2011, 512, 208-210.	2.6	19
61	Structural, optoelectronic, infrared and Raman spectra of orthorhombic SrSnO3 from DFT calculations. Journal of Solid State Chemistry, 2011, 184, 921-928.	2.9	85
62	Charge transport in fibrous/not fibrous Î±3-helical and (5Q,7Q)Î±3 variant peptides. Applied Physics Letters, 2011, 98, .	3.3	10
63	Structural, electronic and optical properties of orthorhombic <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si0047.gif" overflow="scroll"><mml:msub><mml:mrow><mml:mi>CdGeO</mml:mi></mml:mrow><mml:mrow><mml:mn>3</mml:mn></mml:mrow></mml:msub></mml:math> from first principles calculations. Journal of Solid State Chemistry, 2010, 183, 437-443.	2.9	7
64	Graphene Nanoflakes: Thermal Stability, Infrared Signatures, and Potential Applications in the Field of Spintronics and Optical Nanodevices. Journal of Physical Chemistry C, 2010, 114, 17472-17485.	3.1	89
65	Structural, electronic and optical properties of ilmenite and perovskite CdSnO₃from DFT calculations. Journal of Physics Condensed Matter, 2010, 22, 435801.	1.8	20
66	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si24.gif" display="inline" overflow="scroll"><mml:mrow><mml:msub><mml:mrow><mml:mtext>CdXO</mml:mtext></mml:mrow><mml:mrow><mml:mn>3</mml:mn></mml:mrow></mml:msub></mml:math> (X = C, Si, Ge, Sn, Pb) electronic band structures. Chemical Physics Letters, 2009, 480, 273-277.	2.4	22
67	Triclinic CdSiO₃structural, electronic, and optical properties from first principles calculations. Journal Physics D: Applied Physics, 2009, 42, 155406.	2.8	22
68	Defects in Graphene-Based Twisted Nanoribbons: Structural, Electronic, and Optical Properties. Langmuir, 2009, 25, 4751-4759.	3.5	26
69	C₆₀-derived nanobaskets: stability, vibrational signatures, and molecular trapping. Nanotechnology, 2009, 20, 395701.	2.6	8
70	Band structure anisotropy effects on the ultrafast electron transport in 4H-SiC. Solid State Communications, 2008, 145, 397-400.	1.9	1
71	MÃ¶bius and twisted graphene nanoribbons: Stability, geometry, and electronic properties. Journal of Chemical Physics, 2008, 128, 164719.	3.0	54
72	Adsorption of Ascorbic Acid on the C₆₀ Fullerene. Journal of Physical Chemistry B, 2008, 112, 14267-14272.	2.6	30

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73	First-principles calculations of structural, electronic and optical properties of orthorhombic CaPbO₃. Journal Physics D: Applied Physics, 2008, 41, 065405.	2.8	10
74	Optical absorption and electronic band structure first-principles calculations of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Î±</mml:mi></mml:math>-glycine crystals. Physical Review B, 2008, 77, .	3.2	37
75	Si-SiO2-Si and Si-CaCO3-Si coreâ€“double-shell nanoparticles: Tuning light emission from infrared to ultraviolet. Journal of Applied Physics, 2007, 102, 023712.	2.5	0
76	CaO first-principles electronic properties and MOS device simulation. Journal Physics D: Applied Physics, 2007, 40, 1655-1658.	2.8	12
77	High lattice temperature effects on the ultrafast electron transport in 4Hâ€SiC. Journal of Applied Physics, 2007, 102, 053710.	2.5	1
78	Electronic and optical properties of CaCO₃calcite, and excitons in Si@CaCO₃and CaCO₃@SiO₂core-shell quantum dots. Journal Physics D: Applied Physics, 2007, 40, 5747-5752.	2.8	36
79	Structural, electronic, and optical absorption properties of orthorhombic CaSnO3throughab initiocalculations. Journal of Physics Condensed Matter, 2007, 19, 106214.	1.8	29
80	First-principles calculations of structural, electronic, and optical absorption properties of CaCO3 Vaterite. Chemical Physics Letters, 2007, 435, 59-64.	2.6	60
81	Identification of lamivudine conformers by Raman scattering measurements and quantum chemical calculations. Journal of Pharmaceutical and Biomedical Analysis, 2007, 43, 1885-1889.	2.8	14
82	Ab initio structural, electronic and optical properties of orthorhombic. Journal of Solid State Chemistry, 2007, 180, 974-980.	2.9	20
83	Structural and electronic properties of CaSiO3 triclinic. Chemical Physics Letters, 2006, 427, 113-116.	2.6	26
84	Structural, electronic, and optical properties of CaCO3 aragonite. Chemical Physics Letters, 2006, 430, 293-296.	2.6	38
85	Quantum mechanicalab initiocalculations of the Raman scattering from psoralens. Journal of Physics Condensed Matter, 2006, 18, 8325-8336.	1.8	3
86	Structural and optical properties of CaO. Microelectronics Journal, 2005, 36, 1058-1061.	2.0	19
87	Quantum confinement of carriers in heterostructured GaAs/GaP quantum wires. Microelectronics Journal, 2005, 36, 1049-1051.	2.0	2
88	Carrier confinement in AlGaN non-abrupt heterostructured nanowires. Physica Status Solidi C: Current Topics in Solid State Physics, 2005, 2, 2365-2368.	0.8	1
89	Towards Using Multiferroism in Optoelectronics and Spintronics: Tunneling, Confinement and Optical Properties of Si/BiMnO3 Systems. AIP Conference Proceedings, 2005, , .	0.4	1
90	Molecular Signature in the Photoluminescence of Î±-Glycine, L-Alanine and L-Asparagine Crystals: Detection, ab initio Calculations, and Bio-sensor Applications. AIP Conference Proceedings, 2005, , .	0.4	21

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91	Contribution of the charge image potential to carrier confinement in graded Si-based quantum wells. Brazilian Journal of Physics, 2004, 34, 684-686.	1.4	0
92	Exciton confinement in InGaN/GaN cylindrical quantum wires. Brazilian Journal of Physics, 2004, 34, 702-704.	1.4	13
93	Optical properties of zincblende GaN/BN cylindrical nanowires. Applied Surface Science, 2004, 234, 50-53.	6.1	7
94	Transport Transient of Electrons in Wurtzite InN: The Effect of the Band Structure Anisotropy. Physica Status Solidi C: Current Topics in Solid State Physics, 2003, 0, 368-372.	0.8	1
95	Terahertz complex mobility of hot electrons in 3Câ€“ and 6Hâ€“SiC at high temperature. Journal of Applied Physics, 2002, 91, 5208-5212.	2.5	2
96	AC hot carrier transport in 3C- and 6H-SiC in the terahertz frequency and high lattice temperature regime. Brazilian Journal of Physics, 2002, 32, 442-444.	1.4	0
97	Exciton Confinement in GaN/AlGaN Quantum Wells Enhanced by Non-Abrupt Interfaces. Physica Status Solidi (B): Basic Research, 2002, 234, 730-733.	1.5	0
98	Strong graded interface related piezoelectric polarization weakening effects on exciton confinement in single InxGa1â^'xN/GaN quantum wells. Physica E: Low-Dimensional Systems and Nanostructures, 2002, 13, 1106-1110.	2.7	5
99	The influence of graded interfaces in the electronic spectrum of nanometer silicon dots. Applied Surface Science, 2002, 190, 166-170.	6.1	3
100	Strong exciton energy blue shift in graded wurtzite and zincblende GaN/Al0.2Ga0.8N single quantum wells. Journal of Crystal Growth, 2002, 246, 341-346.	1.5	6
101	Band structure effects on the transient electron transport in wurtzite InN. Journal of Crystal Growth, 2002, 246, 320-324.	1.5	7
102	Ultrafast electron drift velocity overshoot in 3Câ€“SiC. Solid State Communications, 2000, 113, 539-542.	1.9	9
103	High Temperature Effects on the Terahertz Mobility of Hot Electrons in 3C-SiC and 6H-SiC. Materials Science Forum, 2000, 338-342, 773-776.	0.3	0
104	High-temperature effects on the velocity overshoot of hot electrons in 6H- and 3C-SiC. Semiconductor Science and Technology, 1999, 14, 1007-1011.	2.0	4
105	Velocity overshoot in zincblende and wurtzite GaN. Solid State Communications, 1999, 110, 469-472.	1.9	20
106	The effect of high Landau subbands filling on the hot-electron magneto-transport ultrafast transient in InSb. Physica B: Condensed Matter, 1999, 269, 28-33.	2.7	0
107	High-Frequency Electron Mobility in GaN. Physica Status Solidi (B): Basic Research, 1999, 216, 737-742.	1.5	1
108	High temperature behavior of subpicosecond electron transport transient in 3C- and 6H-SiC. Brazilian Journal of Physics, 1999, 29, 785-789.	1.4	3

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109	High-magnetic-field effects on the terahertz mobility of hot electrons inn-type InSb. Physical Review B, 1998, 57, 11872-11874.	3.2	14
110	Doping effects on the high-frequency mobility of minority carriers in p-GaAs. Journal of Applied Physics, 1998, 84, 1405-1407.	2.5	0
111	High magnetic field effects on the ultrafast transport transient of hot electrons in InSb. Applied Physics Letters, 1997, 70, 1879-1881.	3.3	9