

# Ewerton Caetano

## List of Publications by Year in descending order

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111  
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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	Graphene Nanoflakes: Thermal Stability, Infrared Signatures, and Potential Applications in the Field of Spintronics and Optical Nanodevices. <i>Journal of Physical Chemistry C</i> , 2010, 114, 17472-17485.	3.1	89
2	DNA-based nanobiostructured devices: The role of quasiperiodicity and correlation effects. <i>Physics Reports</i> , 2014, 535, 139-209.	25.6	88
3	Structural, optoelectronic, infrared and Raman spectra of orthorhombic SrSnO <sub>3</sub> from DFT calculations. <i>Journal of Solid State Chemistry</i> , 2011, 184, 921-928.	2.9	85
4	Explaining statin inhibition effectiveness of HMG-CoA reductase by quantum biochemistry computations. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 1389-1398.	2.8	61
5	First-principles calculations of structural, electronic, and optical absorption properties of CaCO <sub>3</sub> Vaterite. <i>Chemical Physics Letters</i> , 2007, 435, 59-64.	2.6	60
6	Möbius and twisted graphene nanoribbons: Stability, geometry, and electronic properties. <i>Journal of Chemical Physics</i> , 2008, 128, 164719.	3.0	54
7	Structural and optoelectronic properties, and infrared spectrum of cubic BaSnO <sub>3</sub> from first principles calculations. <i>Journal of Applied Physics</i> , 2012, 112, .	2.5	54
8	Polarized Raman, FTIR and DFT study of Na <sub>2</sub> Ti <sub>3</sub> O <sub>7</sub> microcrystals. <i>Journal of Raman Spectroscopy</i> , 2018, 49, 538-548.	2.5	54
9	Optical absorption and DFT calculations in $L$ -aspartic acid anhydrous crystals: Charge carrier effective masses point to semiconducting behavior. <i>Physical Review B</i> , 2012, 86, .	3.2	51
10	Structural and electronic properties of Sr <sub>x</sub> Ba <sub>1-x</sub> SnO <sub>3</sub> from first principles calculations. <i>Journal of Solid State Chemistry</i> , 2012, 187, 186-194.	2.9	47
11	Anhydrous crystals of DNA bases are wide gap semiconductors. <i>Journal of Chemical Physics</i> , 2011, 134, 175101.	3.0	45
12	Quantum molecular modelling of ibuprofen bound to human serum albumin. <i>RSC Advances</i> , 2015, 5, 49439-49450.	3.6	42
13	Elucidating the high- $k$ insulator $\alpha$ -Al <sub>2</sub> O <sub>3</sub> direct/indirect energy band gap type through density functional theory computations. <i>Chemical Physics Letters</i> , 2015, 637, 172-176.	2.6	40
14	Structural, electronic, and optical properties of CaCO <sub>3</sub> aragonite. <i>Chemical Physics Letters</i> , 2006, 430, 293-296.	2.6	38
15	Structural, electronic and optical properties of monoclinic Na <sub>2</sub> Ti <sub>3</sub> O <sub>7</sub> from density functional theory calculations: A comparison with XRD and optical absorption measurements. <i>Journal of Solid State Chemistry</i> , 2017, 250, 68-74.	2.9	38
16	Optical absorption and electronic band structure first-principles calculations of $L$ -glycine crystals. <i>Physical Review B</i> , 2008, 77, .	3.2	37
17	Antipsychotic Haloperidol Binding to the Human Dopamine D <sub>3</sub> Receptor: Beyond Docking Through QM/MM Refinement Toward the Design of Improved Schizophrenia Medicines. <i>ACS Chemical Neuroscience</i> , 2014, 5, 1041-1054.	3.5	37
18	Electronic and optical properties of CaCO <sub>3</sub> calcite, and excitons in Si@CaCO <sub>3</sub> and CaCO <sub>3</sub> @SiO <sub>2</sub> core-shell quantum dots. <i>Journal of Applied Physics</i> , 2007, 40, 5747-5752.	2.8	36

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19	Quantum biochemistry study of the T3-785 tropocollagen triple-helical structure. <i>Chemical Physics Letters</i> , 2013, 559, 88-93.	2.6	31
20	A quantum biochemistry investigation of willardiine partial agonism in AMPA receptors. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 13092-13103.	2.8	31
21	DFT Calculations with van der Waals Interactions of Hydrated Calcium Carbonate Crystals $\text{CaCO}_3 \cdot n\text{H}_2\text{O}$ : Structural, Electronic, Optical, and Vibrational Properties. <i>Journal of Physical Chemistry A</i> , 2016, 120, 5752-5765.	2.5	31
22	Adsorption of Ascorbic Acid on the $\text{C}_{60}$ Fullerene. <i>Journal of Physical Chemistry B</i> , 2008, 112, 14267-14272.	2.6	30
23	Structural, electronic, and optical absorption properties of orthorhombic $\text{CaSnO}_3$ through ab initio calculations. <i>Journal of Physics Condensed Matter</i> , 2007, 19, 106214.	1.8	29
24	A quantum chemistry investigation of a potential inhibitory drug against the dengue virus. <i>RSC Advances</i> , 2016, 6, 56562-56570.	3.6	28
25	$\alpha$ -Serine Anhydrous Crystals: Structural, Electronic, and Optical Properties by First-Principles Calculations, and Optical Absorption Measurement. <i>Crystal Growth and Design</i> , 2013, 13, 2793-2802.	3.0	27
26	Structural and electronic properties of $\text{CaSiO}_3$ triclinic. <i>Chemical Physics Letters</i> , 2006, 427, 113-116.	2.6	26
27	Defects in Graphene-Based Twisted Nanoribbons: Structural, Electronic, and Optical Properties. <i>Langmuir</i> , 2009, 25, 4751-4759.	3.5	26
28	A quantum biochemistry model of the interaction between the estrogen receptor and the two antagonists used in breast cancer treatment. <i>Computational and Theoretical Chemistry</i> , 2016, 1089, 21-27.	2.5	25
29	Quantum binding energy features of the T3-785 collagen-like triple-helical peptide. <i>RSC Advances</i> , 2017, 7, 2817-2828.	3.6	25
30	Two-Level Adsorption of Ibuprofen on $\text{C}_{60}$ Fullerene for Transdermal Delivery: Classical Molecular Dynamics and Density Functional Theory Computations. <i>Journal of Physical Chemistry C</i> , 2011, 115, 24501-24511.	3.1	24
31	$\langle \text{CdXO}_3 \rangle$ ( $X = \text{C, Si, Ge, Sn, Pb}$ ) electronic band structures. <i>Chemical Physics Letters</i> , 2009, 480, 273-277.	2.6	24
32	Triclinic $\text{CdSiO}_3$ structural, electronic, and optical properties from first principles calculations. <i>Journal Physics D: Applied Physics</i> , 2009, 42, 155406.	2.8	22
33	Assessing the Role of Water on the Electronic Structure and Vibrational Spectra of Monohydrated $\alpha$ -Aspartic Acid Crystals. <i>Crystal Growth and Design</i> , 2013, 13, 4844-4851.	3.0	22
34	Vibrational Spectroscopy and Phonon-Related Properties of the $\alpha$ -Aspartic Acid Anhydrous Monoclinic Crystal. <i>Journal of Physical Chemistry A</i> , 2015, 119, 11791-11803.	2.5	22
35	Molecular Signature in the Photoluminescence of $\beta$ -Glycine, L-Alanine and L-Asparagine Crystals: Detection, ab initio Calculations, and Bio-sensor Applications. <i>AIP Conference Proceedings</i> , 2005, , .	0.4	21
36	Velocity overshoot in zincblende and wurtzite GaN. <i>Solid State Communications</i> , 1999, 110, 469-472.	1.9	20

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37	Ab initio structural, electronic and optical properties of orthorhombic. Journal of Solid State Chemistry, 2007, 180, 974-980.	2.9	20
38	Structural, electronic and optical properties of ilmenite and perovskite CdSnO <sub>3</sub> from DFT calculations. Journal of Physics Condensed Matter, 2010, 22, 435801.	1.8	20
39	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
40	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
41	Energetic description of cilengitide bound to integrin. New Journal of Chemistry, 2017, 41, 11405-11412.	2.8	20
42	Structural and optical properties of CaO. Microelectronics Journal, 2005, 36, 1058-1061.	2.0	19
43	Monoclinic and orthorhombic cysteine crystals are small gap insulators. Chemical Physics Letters, 2011, 512, 208-210.	2.6	19
44	The urokinase plasminogen activator binding to its receptor: a quantum biochemistry description within an in/homogeneous dielectric function framework with application to uPA's PAR peptide inhibitors. Physical Chemistry Chemical Physics, 2020, 22, 3570-3583.	2.8	19
45	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
46	Controlled Release of Nor- $\beta$ -lapachone by PLGA Microparticles: A Strategy for Improving Cytotoxicity against Prostate Cancer Cells. Molecules, 2016, 21, 873.	3.8	17
47	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
48	Computational investigation of the $\beta$ - $\beta$ integrin-collagen triple helix complex interaction. New Journal of Chemistry, 2018, 42, 17115-17125.	2.8	16
49	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
50	High-magnetic-field effects on the terahertz mobility of hot electrons in n-type InSb. Physical Review B, 1998, 57, 11872-11874.	3.2	14
51	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
52	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
53	Phosphate group vibrational signatures of the osteoporosis drug alendronate. Journal of Raman Spectroscopy, 2014, 45, 801-806.	2.5	14
54	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

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55	Rose Bengal incorporated to $\beta$ -cyclodextrin microparticles for photodynamic therapy against the cariogenic microorganism <i>Streptococcus mutans</i> . <i>Photodiagnosis and Photodynamic Therapy</i> , 2019, 25, 111-118.	2.6	14
56	Exciton confinement in InGaN/GaN cylindrical quantum wires. <i>Brazilian Journal of Physics</i> , 2004, 34, 702-704.	1.4	13
57	Four-level levodopa adsorption on C60 fullerene for transdermal and oral administration: a computational study. <i>RSC Advances</i> , 2012, 2, 8306.	3.6	13
58	The DNA electronic specific heat at low temperature: The role of aperiodicity. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2012, 376, 2413-2417.	2.1	13
59	Structural, Electronic, and Optical Properties of Bulk Boric Acid $\alpha$ and $\beta$ Polymorphs: Experiment and Density Functional Theory Calculations. <i>Crystal Growth and Design</i> , 2016, 16, 6631-6640.	3.0	13
60	Improved description of the structural and optoelectronic properties of DNA/RNA nucleobase anhydrous crystals: Experiment and dispersion-corrected density functional theory calculations. <i>Physical Review B</i> , 2017, 96, .	3.2	13
61	Structural and Optoelectronic Properties of the $\alpha$ -, $\beta$ -, and $\gamma$ -Glycine Polymorphs and the Glycine Dihydrate Crystal: A DFT Study. <i>Crystal Growth and Design</i> , 2019, 19, 5204-5217.	3.0	13
62	CaO first-principles electronic properties and MOS device simulation. <i>Journal Physics D: Applied Physics</i> , 2007, 40, 1655-1658.	2.8	12
63	An ab initio explanation of the activation and antagonism strength of an AMPA-sensitive glutamate receptor. <i>RSC Advances</i> , 2013, 3, 14988.	3.6	12
64	Computational electronic structure of the bee killer insecticide imidacloprid. <i>New Journal of Chemistry</i> , 2016, 40, 10353-10362.	2.8	12
65	Conductance of single microRNAs chains related to the autism spectrum disorder. <i>Europhysics Letters</i> , 2014, 107, 68006.	2.0	11
66	First-principles calculations of structural, electronic and optical properties of orthorhombic $\text{CaPbO}_3$ . <i>Journal Physics D: Applied Physics</i> , 2008, 41, 065405.	2.8	10
67	Charge transport in fibrous/not fibrous $\alpha$ -helical and $(5Q,7Q)\alpha$ variant peptides. <i>Applied Physics Letters</i> , 2011, 98, .	3.3	10
68	Optical Absorption of the Antitrypanocidal Drug Benznidazole in Water. <i>Molecules</i> , 2014, 19, 4145-4156.	3.8	10
69	Vibrational Properties of Bulk Boric Acid $\alpha$ and $\beta$ Polymorphs and Their Two-Dimensional Layers: Measurements and Density Functional Theory Calculations. <i>Journal of Physical Chemistry A</i> , 2018, 122, 1312-1325.	2.5	10
70	High magnetic field effects on the ultrafast transport transient of hot electrons in InSb. <i>Applied Physics Letters</i> , 1997, 70, 1879-1881.	3.3	9
71	Ultrafast electron drift velocity overshoot in $3C\text{-SiC}$ . <i>Solid State Communications</i> , 2000, 113, 539-542.	1.9	9
72	Electronic transport in methylated fragments of DNA. <i>Applied Physics Letters</i> , 2015, 107, 203701.	3.3	9

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73	First-generation antipsychotic haloperidol: optical absorption measurement and structural, electronic, and optical properties of its anhydrous monoclinic crystal by first-principle approaches. <i>New Journal of Chemistry</i> , 2018, 42, 13629-13640.	2.8	9
74	C <sub>60</sub> -derived nanobaskets: stability, vibrational signatures, and molecular trapping. <i>Nanotechnology</i> , 2009, 20, 395701.	2.6	8
75	An improved quantum biochemistry description of the glutamate-GluA2 receptor binding within an inhomogeneous dielectric function framework. <i>New Journal of Chemistry</i> , 2017, 41, 6167-6179.	2.8	8
76	Band structure effects on the transient electron transport in wurtzite InN. <i>Journal of Crystal Growth</i> , 2002, 246, 320-324.	1.5	7
77	Optical properties of zincblende GaN/BN cylindrical nanowires. <i>Applied Surface Science</i> , 2004, 234, 50-53.	6.1	7
78	Structural, electronic and optical properties of orthorhombic CdGeO <sub>3</sub> from first principles calculations. <i>Journal of Solid State Chemistry</i> , 2010, 183, 437-443.	2.9	7
79	Strong exciton energy blue shift in graded wurtzite and zincblende GaN/Al <sub>0.2</sub> Ga <sub>0.8</sub> N single quantum wells. <i>Journal of Crystal Growth</i> , 2002, 246, 341-346.	1.5	6
80	Encapsulation of nor- $\hat{1}^2$ -lapachone into poly( $\hat{d}$ , $\hat{l}$ )-lactide-co-glycolide (PLGA) microcapsules: full characterization, computational details and cytotoxic activity against human cancer cell lines. <i>MedChemComm</i> , 2017, 8, 1993-2002.	3.4	6
81	Thermal stability and electronic properties of boron nitride nanoflakes. <i>Journal of Molecular Modeling</i> , 2020, 26, 100.	1.8	6
82	Strong graded interface related piezoelectric polarization weakening effects on exciton confinement in single In <sub>x</sub> Ga <sub>1-x</sub> N/GaN quantum wells. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2002, 13, 1106-1110.	2.7	5
83	Structural, electronic, and optical properties of inhomogeneous Ca <sub>1-x</sub> Mg <sub>x</sub> O alloys. <i>Journal of Applied Physics</i> , 2019, 125, 155102.	2.5	5
84	mTOR-mLST8 interaction: hot spot identification through quantum biochemistry calculations. <i>New Journal of Chemistry</i> , 2020, 44, 20982-20992.	2.8	5
85	High-temperature effects on the velocity overshoot of hot electrons in 6H- and 3C-SiC. <i>Semiconductor Science and Technology</i> , 1999, 14, 1007-1011.	2.0	4
86	Carbon-based nanorings sliding along inner coaxial nanotubes: Möbius topology effects in damping gigahertz oscillations. <i>Journal of Applied Physics</i> , 2014, 116, 124311.	2.5	4
87	Changing the gap type of solid state boric acid by heating: a dispersion-corrected density functional study of $\hat{1}^{\pm}$ , $\hat{1}^2$ , and $\hat{1}^3$ -metaboric acid polymorphs. <i>New Journal of Chemistry</i> , 2017, 41, 15533-15544.	2.8	4
88	Vibrational Modes and Phonon and Thermodynamic Properties of the Metaboric Acid Polymorphs $\hat{1}^{\pm}$ , $\hat{1}^2$ , and $\hat{1}^3$ -(BOH) <sub>3</sub> O <sub>3</sub> within a Density Functional Theory Framework. <i>Journal of Physical Chemistry A</i> , 2018, 122, 7628-7645.	2.5	4
89	Solid state properties of hydroxyurea: Optical absorption measurement and DFT calculations. <i>Journal of Applied Physics</i> , 2019, 125, 134901.	2.5	4
90	Novel Si-C compounds with semiconducting and metallic properties: A DFT study. <i>Computational Materials Science</i> , 2020, 183, 109800.	3.0	4

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91	The influence of graded interfaces in the electronic spectrum of nanometer silicon dots. Applied Surface Science, 2002, 190, 166-170.	6.1	3
92	Quantum mechanicalab initio calculations of the Raman scattering from psoralens. Journal of Physics Condensed Matter, 2006, 18, 8325-8336.	1.8	3
93	Electronic specific heat of an $\alpha$ -helical polypeptide and its biochemical variants. Chemical Physics Letters, 2012, 542, 123-127.	2.6	3
94	High temperature behavior of subpicosecond electron transport transient in 3C- and 6H-SiC. Brazilian Journal of Physics, 1999, 29, 785-789.	1.4	3
95	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
96	Terahertz complex mobility of hot electrons in 3C-SiC and 6H-SiC at high temperature. Journal of Applied Physics, 2002, 91, 5208-5212.	2.5	2
97	Quantum confinement of carriers in heterostructured GaAs/GaP quantum wires. Microelectronics Journal, 2005, 36, 1049-1051.	2.0	2
98	High-Frequency Electron Mobility in GaN. Physica Status Solidi (B): Basic Research, 1999, 216, 737-742.	1.5	1
99	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
100	Carrier confinement in AlGaIn non-abrupt heterostructured nanowires. Physica Status Solidi C: Current Topics in Solid State Physics, 2005, 2, 2365-2368.	0.8	1
101	Towards Using Multiferroism in Optoelectronics and Spintronics: Tunneling, Confinement and Optical Properties of Si/BiMnO <sub>3</sub> Systems. AIP Conference Proceedings, 2005, , .	0.4	1
102	High lattice temperature effects on the ultrafast electron transport in 4H-SiC. Journal of Applied Physics, 2007, 102, 053710.	2.5	1
103	Band structure anisotropy effects on the ultrafast electron transport in 4H-SiC. Solid State Communications, 2008, 145, 397-400.	1.9	1
104	Vibrational spectroscopy and phonon-related properties of monoclinic GABA, a non-proteinogenic inhibitory neurotransmitter amino acid. Journal of Raman Spectroscopy, 2021, 52, 1294-1307.	2.5	1
105	Doping effects on the high-frequency mobility of minority carriers in p-GaAs. Journal of Applied Physics, 1998, 84, 1405-1407.	2.5	0
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 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
108	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

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109	Exciton Confinement in GaN/AlGaIn Quantum Wells Enhanced by Non-Abrupt Interfaces. <i>Physica Status Solidi (B): Basic Research</i> , 2002, 234, 730-733.	1.5	0
110	Contribution of the charge image potential to carrier confinement in graded Si-based quantum wells. <i>Brazilian Journal of Physics</i> , 2004, 34, 684-686.	1.4	0
111	Si-SiO <sub>2</sub> -Si and Si-CaCO <sub>3</sub> -Si core-shell double-shell nanoparticles: Tuning light emission from infrared to ultraviolet. <i>Journal of Applied Physics</i> , 2007, 102, 023712.	2.5	0