Vn Freire

List of Publications by Year
in descending order

319 papers	4,690 citations	117625 34 h-index	189892 50 g-index
320 all docs	320 docs citations	320 times ranked	5165 citing authors

#	Article	IF	Citations
1	Understanding the corrosion inhibition of carbon steel and copper in sulphuric acid medium by amino acids using electrochemical techniques allied to molecular modelling methods. Corrosion Science, 2017, 115, 41-55.	6.6	189
2	Structural, electronic, and optical properties of ZrO2 from ab initio calculations. Journal of Applied Physics, 2006, 100, 104103.	2.5	162
3	Resveratrol prevents social deficits in animal model of autism induced by valproic acid. Neuroscience Letters, 2014, 583, 176-181.	2.1	115
4	Deformation induced martensite in an AISI 301LN stainless steel: characterization and influence on pitting corrosion resistance. Materials Research, 2007, 10, 359-366.	1.3	94
5	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
6	DNA-based nanobiostructured devices: The role of quasiperiodicity and correlation effects. Physics Reports, 2014, 535, 139-209.	25.6	88
7	Structural, optoelectronic, infrared and Raman spectra of orthorhombic SrSnO3 from DFT calculations. Journal of Solid State Chemistry, 2011, 184, 921-928.	2.9	85
8	Explaining statin inhibition effectiveness of HMG-CoA reductase by quantum biochemistry computations. Physical Chemistry Chemical Physics, 2012, 14, 1389-1398.	2.8	61
9	First-principles calculations of structural, electronic, and optical absorption properties of CaCO3 Vaterite. Chemical Physics Letters, 2007, 435, 59-64.	2.6	60
10	Coexistence of triclinic and monoclinic phases in WO3 ceramics. Journal of Raman Spectroscopy, 2000, 31, 451-454.	2.5	58
11	Form of the quantum kinetic-energy operator with spatially varying effective mass. Physical Review B, 1997, 55, 1326-1328.	3.2	54
12	Electronic properties of a quasi-two-dimensional electron gas in semiconductor quantum wells under intense laser fields. Physical Review B, 2004, 70, .	3.2	54
13	MÃ¶bius and twisted graphene nanoribbons: Stability, geometry, and electronic properties. Journal of Chemical Physics, 2008, 128, 164719.	3.0	54
14	Structural and optoelectronic properties, and infrared spectrum of cubic BaSnO3 from first principles calculations. Journal of Applied Physics, 2012, 112, .	2.5	54
15	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
16	Full-relativistic calculations of the SrTiO3 carrier effective masses and complex dielectric function. Applied Physics Letters, 2003, 82, 3074-3076.	3.3	53
17	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
18	Intraband absorption and Stark effect in silicon nanocrystals. Physical Review B, 2005, 72, .	3.2	50

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19	Three-dimensional self-consistent simulation of the charging time response in silicon nanocrystal flash memories. Journal of Applied Physics, 2002, 92, 6182-6187.	2.5	47
20	Structural and electronic properties of SrxBa1â^'xSnO3 from first principles calculations. Journal of Solid State Chemistry, 2012, 187, 186-194.	2.9	47
21	Anhydrous crystals of DNA bases are wide gap semiconductors. Journal of Chemical Physics, 2011, 134, 175101.	3.0	45
22	Production and characterization of the cashew (Anacardium occidentale L.) peduncle bagasse ashes. Journal of Food Engineering, 2007, 79, 1432-1437.	5.2	44
23	Quantum molecular modelling of ibuprofen bound to human serum albumin. RSC Advances, 2015, 5, 49439-49450.	3.6	42
24	Interface-related exciton-energy blueshift inGaN/AlxGa1â^'xNzinc-blende and wurtzite single quantum wells. Physical Review B, 1999, 60, 5705-5713.	3.2	41
25	Slab lenses from simple anisotropic media. Physical Review B, 2005, 72, .	3.2	40
26	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
27	Structural, electronic, and optical properties of CaCO3 aragonite. Chemical Physics Letters, 2006, 430, 293-296.	2.6	38
28	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
29	Effective masses and complex dielectric function of cubic HfO2. Applied Physics Letters, 2004, 85, 5022-5024.	3.3	37
30	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
31	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
32	RA Differentiation Enhances Dopaminergic Features, Changes Redox Parameters, and Increases Dopamine Transporter Dependency in 6-Hydroxydopamine-Induced Neurotoxicity in SH-SY5Y Cells. Neurotoxicity Research, 2017, 31, 545-559.	2.7	37
33	Phase transition in WO3microcrystals obtained by sintering process. Journal of Raman Spectroscopy, 2001, 32, 695-699.	2.5	36
34	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
35	Pressure effects in the Raman spectrum ofWO3microcrystals. Physical Review B, 2000, 62, 3699-3703.	3.2	35
36	Crystal structure of a lectin from Canavalia maritima (ConM) in complex with trehalose and maltose reveals relevant mutation in ConA-like lectins. Journal of Structural Biology, 2006, 154, 280-286.	2.8	34

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37	Acoustic phonon transmission spectra in piezoelectric AlN/GaN Fibonacci phononic crystals. European Physical Journal B, 2007, 58, 379-387.	1.5	34
38	Evidence of magnetic polaronic states inLa0.70Sr0.30Mn1â^'xFexO3manganites. Physical Review B, 2003, 67, .	3.2	33
39	Role of Cu, Ni and Co metals in the acidic and redox properties of Mo catalysts supported on Al₂O₃ spheres for glycerol conversion. Catalysis Science and Technology, 2016, 6, 4986-5002.	4.1	33
40	Velocity overshoot onset in nitride semiconductors. Applied Physics Letters, 2000, 76, 1893-1895.	3.3	32
41	Quantum biochemistry study of the T3-785 tropocollagen triple-helical structure. Chemical Physics Letters, 2013, 559, 88-93.	2.6	31
42	A quantum biochemistry investigation of willardiine partial agonism in AMPA receptors. Physical Chemistry Chemical Physics, 2015, 17, 13092-13103.	2.8	31
43	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
44	Adsorption of Ascorbic Acid on the C₆₀ Fullerene. Journal of Physical Chemistry B, 2008, 112, 14267-14272.	2.6	30
45	An improved description of the dielectric breakdown in oxides based on a generalized Weibull distribution. Physica A: Statistical Mechanics and Its Applications, 2006, 361, 209-215.	2.6	29
46	Structural, electronic, and optical absorption properties of orthorhombic CaSnO3throughab initiocalculations. Journal of Physics Condensed Matter, 2007, 19, 106214.	1.8	29
47	Ultrafast mobility in photoinjected polar semiconductors. Physical Review B, 1989, 39, 13264-13275.	3.2	28
48	A quantum chemistry investigation of a potential inhibitory drug against the dengue virus. RSC Advances, 2016, 6, 56562-56570.	3.6	28
49	Production in Pichia pastoris, antifungal activity and crystal structure of a class I chitinase from cowpea (Vigna unguiculata): Insights into sugar binding mode and hydrolytic action. Biochimie, 2017, 135, 89-103.	2.6	28
50	<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
51	Structural and electronic properties of CaSiO3 triclinic. Chemical Physics Letters, 2006, 427, 113-116.	2.6	26
52	Crystal structure of Dioclea rostrata lectin: Insights into understanding the pH-dependent dimer-tetramer equilibrium and the structural basis for carbohydrate recognition in Diocleinae lectins. Journal of Structural Biology, 2008, 164, 177-182.	2.8	26
53	Defects in Graphene-Based Twisted Nanoribbons: Structural, Electronic, and Optical Properties. Langmuir, 2009, 25, 4751-4759.	3.5	26
54	Coal Fly Ash Ceramics: Preparation, Characterization, and Use in the Hydrolysis of Sucrose. Scientific World Journal, The, 2014, 2014, 1-7.	2.1	26

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55	Carbon fiber/epoxy composites: effect of zinc sulphide coated carbon nanotube on thermal and mechanical properties. Polymer Bulletin, 2018, 75, 1619-1633.	3.3	26
56	Immobilization of urease on vapour phase stain etched porous silicon. Process Biochemistry, 2007, 42, 429-433.	3.7	25
57	Angiotensin Converting Enzyme Regulates Cell Proliferation and Migration. PLoS ONE, 2016, 11, e0165371.	2.5	25
58	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
59	Quantum binding energy features of the T3-785 collagen-like triple-helical peptide. RSC Advances, 2017, 7, 2817-2828.	3.6	25
60	Nonlinear transport properties of III-nitrides in electric field. Journal of Applied Physics, 2005, 98, 043702.	2.5	24
61	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
62	Nanoencapsulation of benznidazole in calcium carbonate increases its selectivity to Trypanosoma cruzi. Parasitology, 2018, 145, 1191-1198.	1.5	24
63	Microstructural and electrical properties of sintered tungsten trioxide. Journal of Materials Science, 1999, 34, 1031-1035.	3.7	23
64	Antimicrobial effect of Dinoponera quadriceps (Hymenoptera: Formicidae) venom against Staphylococcus aureus strains. Journal of Applied Microbiology, 2014, 117, 390-396.	3.1	23
65	Carbon steel corrosion inhibition in acid medium by imidazole-based molecules: Experimental and molecular modelling approaches. Journal of Molecular Liquids, 2021, 326, 115330.	4.9	23
66	Hole mobility in zincblende câ€“GaN. Journal of Applied Physics, 2004, 95, 4914-4917.	2.5	22
67	<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</ (X = C, Si, Ge, Sn, Pb) electronic band structures. Chemical Physics Letters, 2009, 480, 273-277.	2.6	22
68	Triclinic CdSiO₃structural, electronic, and optical properties from first principles calculations. Journal Physics D: Applied Physics, 2009, 42, 155406.	2.8	22
69	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
70	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
71	Simple synthesis of Al2O3 sphere composite from hybrid process with improved thermal stability for catalytic applications. Materials Chemistry and Physics, 2015, 160, 119-130.	4.0	22
72	Purification, Biochemical Characterization, and Amino Acid Sequence of a Novel Type of Lectin from Aplysia dactylomela Eggs with Antibacterial/Antibiofilm Potential. Marine Biotechnology, 2017, 19, 49-64.	2.4	22

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73	Hot Electron Dynamics in Zincblende and Wurtzite GaN. Physica Status Solidi (B): Basic Research, 1999, 216, 35-39.	1.5	21
74	Confinement of two-dimensional excitons in a nonhomogeneous magnetic field. Physical Review B, 2000, 61, 2895-2903.	3.2	21
75	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
76	Trypanocidal activity of mastoparan from Polybia paulista wasp venom by interaction with TcGAPDH. Toxicon, 2017, 137, 168-172.	1.6	21
77	Velocity overshoot in zincblende and wurtzite GaN. Solid State Communications, 1999, 110, 469-472.	1.9	20
78	Urbachâ€™s tail in III-nitrides under an electric field. Journal of Applied Physics, 2001, 90, 1879-1882.	2.5	20
79	Hot-phonon bottleneck in the photoinjected plasma in GaN. Applied Physics Letters, 2003, 82, 2455-2457.	3.3	20
80	Ab initio structural, electronic and optical properties of orthorhombic. Journal of Solid State Chemistry, 2007, 180, 974-980.	2.9	20
81	Structural, electronic and optical properties of ilmenite and perovskite CdSnO₃from DFT calculations. Journal of Physics Condensed Matter, 2010, 22, 435801.	1.8	20
82	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
83	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
84	Energetic description of cilengitide bound to integrin. New Journal of Chemistry, 2017, 41, 11405-11412.	2.8	20
85	Effects of crystallographic orientations on the charging time in silicon nanocrystal flash memories. Applied Physics Letters, 2003, 82, 2685-2687.	3.3	19
86	Structural and optical properties of CaO. Microelectronics Journal, 2005, 36, 1058-1061.	2.0	19
87	Nonlinear transport properties of doped III-N and GaAs polar semiconductors: A comparison. Journal of Applied Physics, 2005, 98, 043703.	2.5	19
88	Monoclinic and orthorhombic cysteine crystals are small gap insulators. Chemical Physics Letters, 2011, 512, 208-210.	2.6	19
89	Ribosomal RNAâ€“Aminoglycoside Hygromycin B Interaction Energy Calculation within a Density Functional Theory Framework. Journal of Physical Chemistry B, 2019, 123, 6421-6429.	2.6	19
90	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

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91	Band Structure Derived Properties of HfO2 from First Principles Calculations. AIP Conference Proceedings, 2005, , .	0.4	18
92	Hole-versus electron-based operations in SiGe nanocrystal nonvolatile memories. Applied Physics Letters, 2007, 90, 223504.	3.3	18
93	The quantum biophysics of the isoniazid adduct NADH binding to its InhA reductase target. New Journal of Chemistry, 2014, 38, 2946.	2.8	18
94	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
95	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
96	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
97	Electron mobility in nitride materials. Brazilian Journal of Physics, 2002, 32, 439-441.	1.4	17
98	Computational investigation of the Î±₂Î²₁integrinâ€“collagen triple helix complex interaction. New Journal of Chemistry, 2018, 42, 17115-17125.	2.8	16
99	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
100	Structural basis of ConM binding with resveratrol, an anti-inflammatory and antioxidant polyphenol. International Journal of Biological Macromolecules, 2015, 72, 1136-1142.	7.5	15
101	Quantum Biochemistry Description of the Human Dopamine D3 Receptor in Complex with the Selective Antagonist Eticlopride. Journal of Proteomics and Bioinformatics, 2012, 05, .	0.4	15
102	High-magnetic-field effects on the terahertz mobility of hot electrons inn-type InSb. Physical Review B, 1998, 57, 11872-11874.	3.2	14
103	Smooth interface effects on the Raman scattering in zinc-blende AlN/GaN superlattices. Physical Review B, 2000, 61, 13060-13063.	3.2	14
104	Transient transport in III-nitrides: interplay of momentum and energy relaxation times. Journal of Physics Condensed Matter, 2007, 19, 346214.	1.8	14
105	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
106	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
107	Phosphate group vibrational signatures of the osteoporosis drug alendronate. Journal of Raman Spectroscopy, 2014, 45, 801-806.	2.5	14
108	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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109	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
110	Highâ€field transport transient of minority carriers inpâ€GaAs. Applied Physics Letters, 1991, 59, 558-560.	3.3	13
111	Exciton confinement in InGaN/GaN cylindrical quantum wires. Brazilian Journal of Physics, 2004, 34, 702-704.	1.4	13
112	Crystallization and preliminary X-ray diffraction analysis of the lectin fromCanavalia gladiataseeds. Acta Crystallographica Section D: Biological Crystallography, 2004, 60, 1493-1495.	2.5	13
113	Correlation betweenEnterococcus faecalisBiofilms Development Stage and Quantitative Surface Roughness Using Atomic Force Microscopy. Microscopy and Microanalysis, 2008, 14, 150-158.	0.4	13
114	Four-level levodopa adsorption on C60 fullerene for transdermal and oral administration: a computational study. RSC Advances, 2012, 2, 8306.	3.6	13
115	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
116	Direct electrochemical analysis of dexamethasone endocrine disruptor in raw natural waters. Journal of the Brazilian Chemical Society, 2012, 23, 110-119.	0.6	13
117	Immobilized invertase studies on glassâ€“ceramic support from coal fly ashes. Chemical Engineering Journal, 2013, 214, 91-96.	12.7	13
118	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
119	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
120	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
121	Resonant peaks in the transmission coefficient of compositionally nonabrupt GaAs/AlxGa1âˆ’xAs heterojunctions. Superlattices and Microstructures, 1992, 11, 17-22.	3.1	12
122	Fine structure of excitons in a quantum well in the presence of a nonhomogeneous magnetic field. Physical Review B, 2000, 62, 7316-7324.	3.2	12
123	Theoretical investigation of excitons in type-I and type-IISiâˆ•Si1âˆ’xGexquantum wires. Physical Review B, 2006, 74, .	3.2	12
124	CaO first-principles electronic properties and MOS device simulation. Journal Physics D: Applied Physics, 2007, 40, 1655-1658.	2.8	12
125	The new flow system approach in packed bed reactor applicable for immobilized enzyme. Journal of Molecular Catalysis B: Enzymatic, 2012, 79, 1-7.	1.8	12
126	An ab initio explanation of the activation and antagonism strength of an AMPA-sensitive glutamate receptor. RSC Advances, 2013, 3, 14988.	3.6	12

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127	Cubic superparamagnetic nanoparticles of NiFe2O4 via fast microwave heating. Journal of Nanoparticle Research, 2014, 16, 1.	1.9	12
128	Computational electronic structure of the bee killer insecticide imidacloprid. New Journal of Chemistry, 2016, 40, 10353-10362.	2.8	12
129	Cloning of cDNA sequences encoding cowpea (Vigna unguiculata) vicilins: Computational simulations suggest a binding mode of cowpea vicilins to chitin oligomers. International Journal of Biological Macromolecules, 2018, 117, 565-573.	7.5	12
130	Intraband absorption in silicon nanocrystals: The combined effect of shape and crystal orientation. Applied Physics Letters, 2005, 87, 031913.	3.3	11
131	Conductance of single microRNAs chains related to the autism spectrum disorder. Europhysics Letters, 2014, 107, 68006.	2.0	11
132	Modeling of laccase inhibition by formetanate pesticide using theoretical approaches. Bioelectrochemistry, 2016, 108, 46-53.	4.6	11
133	Localization and fractal spectra of optical phonon modes in quasiperiodic structures. Physica A: Statistical Mechanics and Its Applications, 2005, 349, 259-270.	2.6	10
134	First-principles calculations of structural, electronic and optical properties of orthorhombic CaPbO₃. Journal Physics D: Applied Physics, 2008, 41, 065405.	2.8	10
135	Charge transport in fibrous/not fibrous Î±3-helical and (5Q,7Q)Î±3 variant peptides. Applied Physics Letters, 2011, 98, .	3.3	10
136	Sensitive voltammetric responses and mechanistic insights into the determination of residue levels of endosulfan in fresh foodstuffs and raw natural waters. Microchemical Journal, 2013, 110, 40-47.	4.5	10
137	Dimethomorph electrooxidation: Analytical determination in grape-derived samples and mechanistic aspects. Electrochimica Acta, 2013, 107, 350-357.	5.2	10
138	Optical Absorption of the Antitrypanocidal Drug Benznidazole inWater. Molecules, 2014, 19, 4145-4156.	3.8	10
139	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
140	High magnetic field effects on the ultrafast transport transient of hot electrons in InSb. Applied Physics Letters, 1997, 70, 1879-1881.	3.3	9
141	Ultrafast electron drift velocity overshoot in 3Câ€“SiC. Solid State Communications, 2000, 113, 539-542.	1.9	9
142	Effect of ageing on x-ray induced dopant passivation in MOS capacitors. Semiconductor Science and Technology, 2000, 15, 794-798.	2.0	9
143	A Raman scattering-based method to probe the carrier drift velocity in semiconductors: Application to gallium nitride. Applied Physics Letters, 2004, 85, 4055-4057.	3.3	9
144	Electronic transport in methylated fragments of DNA. Applied Physics Letters, 2015, 107, 203701.	3.3	9

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145	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
146	Quantum biochemistry in cancer immunotherapy: New insights about CTLA-4/ipilimumab and design of ipilimumab-derived peptides with high potential in cancer treatment. Molecular Immunology, 2020, 127, 203-211.	2.2	9
147	ACE2-derived peptides interact with the RBD domain of SARS-CoV-2 spike glycoprotein, disrupting the interaction with the human ACE2 receptor. Journal of Biomolecular Structure and Dynamics, 2022, 40, 5493-5506.	3.5	9
148	Transmission coefficient of electrons through a single graded barrier. Physical Review B, 1993, 48, 8446-8449.	3.2	8
149	Time evolution of SiO2/Si interface defects and dopant passivation in MOS capacitors. Microelectronic Engineering, 2000, 51-52, 567-574.	2.4	8
150	Strong interface localization of phonons in nonabrupt InN/GaN superlattices. Physical Review B, 2001, 64, .	3.2	8
151	Interface-related effects on confined excitons in GaAs/AlxGa1â^'xAs single quantum wells. Applied Surface Science, 2002, 190, 191-194.	6.1	8
152	Mobility in n-doped wurtzite III-Nitrides. Materials Research, 2003, 6, 01-04.	1.3	8
153	Two different incorporation sites of manganese in single-crystalline monohydratedL-asparagine studied by electron paramagnetic resonance. Physical Review B, 2007, 75, .	3.2	8
154	C₆₀-derived nanobaskets: stability, vibrational signatures, and molecular trapping. Nanotechnology, 2009, 20, 395701.	2.6	8
155	Performance of invertase immobilized on glassâ€"ceramic supports in batch bioreactor. Chemical Engineering Journal, 2012, 187, 341-350.	12.7	8
156	Electrochemical and Monte Carlo studies of self-assembled trans-[Fe(cyclam)(NCS)2]+ complex ion on gold surface as electrochemical sensor for nitric oxide. Electrochimica Acta, 2013, 91, 1-10.	5.2	8
157	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
158	CO2 role on the glycerol conversion over catalyst containing CaO-SiO2 doped with Ag and Pt. Catalysis Today, 2020, 344, 199-211.	4.4	8
159	Quantum biochemistry, molecular docking, and dynamics simulation revealed synthetic peptides induced conformational changes affecting the topology of the catalytic site of SARS-CoV-2 main protease. Journal of Biomolecular Structure and Dynamics, 2022, 40, 8925-8937.	3.5	8
160	Optical properties of ellipsoidal CdSe quantum dots. Brazilian Journal of Physics, 2006, 36, 438-439.	1.4	8
161	Electron transmission through a single nonabrupt GaAs/AlxGa1â^'xAs barrier subjected to an electric field. Physical Review B, 1995, 52, 5777-5780.	3.2	7
162	Emission spectrum in driven two-level systems. Physical Review A, 1998, 58, 1531-1536.	2.5	7

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163	Sign inversion of the Stark shift in single non-abrupt GaAs/AlxGa1-xAs quantum wells. Journal of Physics Condensed Matter, 1999, 11, 5593-5602.	1.8	7
164	Band structure of a cylindrical GaAs/AlxGa1âˆ’xAs superwire. Superlattices and Microstructures, 1999, 25, 221-225.	3.1	7
165	Band structure effects on the transient electron transport in wurtzite InN. Journal of Crystal Growth, 2002, 246, 320-324.	1.5	7
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