

# Vn Freire

## List of Publications by Year in descending order

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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	ACE2-derived peptides interact with the RBD domain of SARS-CoV-2 spike glycoprotein, disrupting the interaction with the human ACE2 receptor. <i>Journal of Biomolecular Structure and Dynamics</i> , 2022, 40, 5493-5506.	3.5	9
2	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. <i>Journal of Biomolecular Structure and Dynamics</i> , 2022, 40, 8925-8937.	3.5	8
3	Gallic acid leads to cell death of <i>Candida albicans</i> by the apoptosis mechanism. <i>Future Microbiology</i> , 2022, 17, 599-606.	2.0	7
4	Optical absorption measurements and optoelectronic DFT calculations for ethanol solvated quercetin and anhydrous/hydrated quercetin crystals. <i>Journal of Solid State Chemistry</i> , 2022, 312, 123242.	2.9	3
5	<i>In silico</i> approach of modified melanoma peptides and their immunotherapeutic potential. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 2836-2845.	2.8	3
6	Carbon steel corrosion inhibition in acid medium by imidazole-based molecules: Experimental and molecular modelling approaches. <i>Journal of Molecular Liquids</i> , 2021, 326, 115330.	4.9	23
7	Vibrational spectroscopy and phonon-related properties of monoclinic GABA, a non-proteinogenic inhibitory neurotransmitter amino acid. <i>Journal of Raman Spectroscopy</i> , 2021, 52, 1294-1307.	2.5	1
8	Computational approach, scanning electron and fluorescence microscopies revealed insights into the action mechanisms of anticandidal peptide Mo-CBP3-PepIII. <i>Life Sciences</i> , 2021, 281, 119775.	4.3	6
9	New ethionamide boosters and EthR2: structural and energetic analysis. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 23233-23241.	2.8	4
10	Insulin degludec and glutamine dipeptide modify glucose homeostasis and liver metabolism in diabetic mice undergoing insulin-induced hypoglycemia. <i>Journal of Applied Biomedicine</i> , 2021, 19, 210-219.	1.7	2
11	CO <sub>2</sub> role on the glycerol conversion over catalyst containing CaO-SiO <sub>2</sub> doped with Ag and Pt. <i>Catalysis Today</i> , 2020, 344, 199-211.	4.4	8
12	mTOR-mLST8 interaction: hot spot identification through quantum biochemistry calculations. <i>New Journal of Chemistry</i> , 2020, 44, 20982-20992.	2.8	5
13	Quantum biochemistry in cancer immunotherapy: New insights about CTLA-4/ipilimumab and design of ipilimumab-derived peptides with high potential in cancer treatment. <i>Molecular Immunology</i> , 2020, 127, 203-211.	2.2	9
14	Novel Si-C compounds with semiconducting and metallic properties: A DFT study. <i>Computational Materials Science</i> , 2020, 183, 109800.	3.0	4
15	Betaine-loaded CaCO <sub>3</sub> microparticles improve survival of vitrified feline preantral follicles through higher mitochondrial activity and decreased reactive oxygen species. <i>Reproduction, Fertility and Development</i> , 2020, 32, 531.	0.4	4
16	Crystal structure and specific location of a germin-like protein with proteolytic activity from <i>Thevetia peruviana</i> . <i>Plant Science</i> , 2020, 298, 110590.	3.6	2
17	Study of the vibrational properties of haloperidol under high-pressure. <i>Vibrational Spectroscopy</i> , 2020, 109, 103103.	2.2	1
18	The urokinase plasminogen activator binding to its receptor: a quantum biochemistry description within an inhomogeneous dielectric function framework with application to uPA-uPAR peptide inhibitors. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 3570-3583.	2.8	19

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19	Antitumor Potential of the Isoflavonoids (+)- and (±)-2,3,9-Trimethoxypterocarpan: Mechanism-of-Action Studies. ACS Medicinal Chemistry Letters, 2020, 11, 1274-1280.	2.8	6
20	Structural and Optoelectronic Properties of the $\hat{1}\pm$ , $\hat{1}^2$ -, and $\hat{1}^3$ -Glycine Polymorphs and the Glycine Dihydrate Crystal: A DFT Study. Crystal Growth and Design, 2019, 19, 5204-5217.	3.0	13
21	Ribosomal RNA–Aminoglycoside Hygromycin B Interaction Energy Calculation within a Density Functional Theory Framework. Journal of Physical Chemistry B, 2019, 123, 6421-6429.	2.6	19
22	Structural, electronic, and optical properties of inhomogeneous $\text{Ca}_{1-x}\text{Mg}_x\text{O}$ alloys. Journal of Applied Physics, 2019, 125, 155102.	2.5	5
23	Solid state properties of hydroxyurea: Optical absorption measurement and DFT calculations. Journal of Applied Physics, 2019, 125, 134901.	2.5	4
24	MOLECULAR FRACTIONATION WITH CONJUGATE CAPS STUDY OF THE INTERACTION OF THE ANACARDIC ACID WITH THE ACTIVE SITE OF TRYPANOSOMA CRUZI GAPDH ENZYME: A QUANTUM INVESTIGATION. Asian Journal of Pharmaceutical and Clinical Research, 2019, , 183-189.	0.3	1
25	Rose Bengal incorporated to $\hat{1}$ -cyclodextrin microparticles for photodynamic therapy against the cariogenic microorganism Streptococcus mutans. Photodiagnosis and Photodynamic Therapy, 2019, 25, 111-118.	2.6	14
26	Nanoencapsulation of benzimidazole in calcium carbonate increases its selectivity to <i>Trypanosoma cruzi</i> . Parasitology, 2018, 145, 1191-1198.	1.5	24
27	Vibrational Properties of Bulk Boric Acid $2A$ and $3TP$ Polymorphs and Their Two-Dimensional Layers: Measurements and Density Functional Theory Calculations. Journal of Physical Chemistry A, 2018, 122, 1312-1325.	2.5	10
28	Polarized Raman, $\langle \text{FTIR} \rangle$ and $\langle \text{DFT} \rangle$ study of $\langle \text{Na}_2\text{Ti}_3\text{O}_7 \rangle$ microcrystals. Journal of Raman Spectroscopy, 2018, 49, 538-548.	2.5	54
29	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
30	Copper promoter effect on acid–base and redox sites of $\text{Fe/Al}_2\text{O}_3$ catalysts and their role in ethanol–acetone mixture conversion. Catalysis Science and Technology, 2018, 8, 443-458.	4.1	6
31	Computational investigation of the $\hat{1}\pm$ and $\hat{1}^2$ integrin–collagen triple helix complex interaction. New Journal of Chemistry, 2018, 42, 17115-17125.	2.8	16
32	Vibrational Modes and Phonon and Thermodynamic Properties of the Metaboric Acid Polymorphs $\hat{1}\pm$ , $\hat{1}^2$ -, and $\hat{1}^3$ -(BOH) $_3\text{O}_3$ within a Density Functional Theory Framework. Journal of Physical Chemistry A, 2018, 122, 7628-7645.	2.5	4
33	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
34	Interaction energy profile for diphenyl diselenide in complex with $\hat{1}$ -aminolevulinic acid dehydratase enzyme using quantum calculations and a molecular fragmentation method. Computational Toxicology, 2018, 7, 9-19.	3.3	5
35	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
36	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

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37	Explaining urokinase type plasminogen activator inhibition by amino-5-hydroxybenzimidazole and two naphthamidine-based compounds through quantum biochemistry. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 22818-22830.	2.8	4
38	Purification, Biochemical Characterization, and Amino Acid Sequence of a Novel Type of Lectin from <i>Aplysia dactylomela</i> Eggs with Antibacterial/Antibiofilm Potential. <i>Marine Biotechnology</i> , 2017, 19, 49-64.	2.4	22
39	RA Differentiation Enhances Dopaminergic Features, Changes Redox Parameters, and Increases Dopamine Transporter Dependency in 6-Hydroxydopamine-Induced Neurotoxicity in SH-SY5Y Cells. <i>Neurotoxicity Research</i> , 2017, 31, 545-559.	2.7	37
40	Quantum binding energy features of the T3-785 collagen-like triple-helical peptide. <i>RSC Advances</i> , 2017, 7, 2817-2828.	3.6	25
41	Production in <i>Pichia pastoris</i> , antifungal activity and crystal structure of a class I chitinase from cowpea ( <i>Vigna unguiculata</i> ): Insights into sugar binding mode and hydrolytic action. <i>Biochimie</i> , 2017, 135, 89-103.	2.6	28
42	cDNA cloning, molecular modeling and docking calculations of L-type lectins from <i>Swartzia simplex</i> var. <i>grandiflora</i> (Leguminosae, Papilionoideae), a member of the tribe Swartzieae. <i>Phytochemistry</i> , 2017, 139, 60-71.	2.9	6
43	The vibrational properties of the bee-killer imidacloprid insecticide: A molecular description. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2017, 185, 245-255.	3.9	20
44	An improved quantum biochemistry description of the glutamateâ€“GluA2 receptor binding within an inhomogeneous dielectric function framework. <i>New Journal of Chemistry</i> , 2017, 41, 6167-6179.	2.8	8
45	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
46	Energetic description of cilengitide bound to integrin. <i>New Journal of Chemistry</i> , 2017, 41, 11405-11412.	2.8	20
47	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
48	Encapsulation of nor- $\beta$ -lapachone into poly( $\epsilon$ -CL, 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
49	Trypanocidal activity of mastoparan from <i>Polybia paulista</i> wasp venom by interaction with TcGAPDH. <i>Toxicon</i> , 2017, 137, 168-172.	1.6	21
50	Changing the gap type of solid state boric acid by heating: a dispersion-corrected density functional study of $I^{\pm}$ , $I^{2-}$ , and $I^{3-}$ metaboric acid polymorphs. <i>New Journal of Chemistry</i> , 2017, 41, 15533-15544.	2.8	4
51	Understanding the corrosion inhibition of carbon steel and copper in sulphuric acid medium by amino acids using electrochemical techniques allied to molecular modelling methods. <i>Corrosion Science</i> , 2017, 115, 41-55.	6.6	189
52	Controlled Release of Nor- $\beta$ -lapachone by PLGA Microparticles: A Strategy for Improving Cytotoxicity against Prostate Cancer Cells. <i>Molecules</i> , 2016, 21, 873.	3.8	17
53	Angiotensin Converting Enzyme Regulates Cell Proliferation and Migration. <i>PLoS ONE</i> , 2016, 11, e0165371.	2.5	25
54	Role of Cu, Ni and Co metals in the acidic and redox properties of Mo catalysts supported on Al <sub>2</sub> O <sub>3</sub> spheres for glycerol conversion. <i>Catalysis Science and Technology</i> , 2016, 6, 4986-5002.	4.1	33

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55	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
56	Structural, Electronic, and Optical Properties of Bulk Boric Acid $\alpha$ and $\beta$ Polymorphs: Experiment and Density Functional Theory Calculations. Crystal Growth and Design, 2016, 16, 6631-6640.	3.0	13
57	Explaining RANKL inhibition by OPG through quantum biochemistry computations and insights into peptide-design for the treatment of osteoporosis. RSC Advances, 2016, 6, 84926-84942.	3.6	7
58	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
59	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. Journal of Physical Chemistry A, 2016, 120, 5752-5765.	2.5	31
60	Computational electronic structure of the bee killer insecticide imidacloprid. New Journal of Chemistry, 2016, 40, 10353-10362.	2.8	12
61	A quantum chemistry investigation of a potential inhibitory drug against the dengue virus. RSC Advances, 2016, 6, 56562-56570.	3.6	28
62	Modeling of laccase inhibition by formetanate pesticide using theoretical approaches. Bioelectrochemistry, 2016, 108, 46-53.	4.6	11
63	Elucidating the high-k insulator $\alpha$ - $\text{Al}_2\text{O}_3$ direct/indirect energy band gap type through density functional theory computations. Chemical Physics Letters, 2015, 637, 172-176.	2.6	40
64	Electronic transport in methylated fragments of DNA. Applied Physics Letters, 2015, 107, 203701.	3.3	9
65	Quantum molecular modelling of ibuprofen bound to human serum albumin. RSC Advances, 2015, 5, 49439-49450.	3.6	42
66	Vibrational Spectroscopy and Phonon-Related Properties of the $\alpha$ -Aspartic Acid Anhydrous Monoclinic Crystal. Journal of Physical Chemistry A, 2015, 119, 11791-11803.	2.5	22
67	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
68	A quantum biochemistry investigation of willardiine partial agonism in AMPA receptors. Physical Chemistry Chemical Physics, 2015, 17, 13092-13103.	2.8	31
69	Simple synthesis of $\text{Al}_2\text{O}_3$ sphere composite from hybrid process with improved thermal stability for catalytic applications. Materials Chemistry and Physics, 2015, 160, 119-130.	4.0	22
70	Coal Fly Ash Ceramics: Preparation, Characterization, and Use in the Hydrolysis of Sucrose. Scientific World Journal, The, 2014, 2014, 1-7.	2.1	26
71	Optical Absorption of the Antitrypanocidal Drug Benznidazole in Water. Molecules, 2014, 19, 4145-4156.	3.8	10
72	Conductance of single microRNAs chains related to the autism spectrum disorder. Europhysics Letters, 2014, 107, 68006.	2.0	11

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73	Cubic superparamagnetic nanoparticles of NiFe <sub>2</sub> O <sub>4</sub> via fast microwave heating. Journal of Nanoparticle Research, 2014, 16, 1.	1.9	12
74	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
75	Phosphate group vibrational signatures of the osteoporosis drug alendronate. Journal of Raman Spectroscopy, 2014, 45, 801-806.	2.5	14
76	262 Improved cytotoxic activity of Nor- $\beta$ -lapachone-loaded PLGA microcapsules in PC3M prostate cancer cell line. European Journal of Cancer, 2014, 50, 87.	2.8	0
77	DNA-based nanobiostructured devices: The role of quasiperiodicity and correlation effects. Physics Reports, 2014, 535, 139-209.	25.6	88
78	The quantum biophysics of the isoniazid adduct NADH binding to its InhA reductase target. New Journal of Chemistry, 2014, 38, 2946.	2.8	18
79	Carbon-based nanorings sliding along inner coaxial nanotubes: Möbius topology effects in damping gigahertz oscillations. Journal of Applied Physics, 2014, 116, 124311.	2.5	4
80	Exploiting the Reduction of Haloperidol: Electrochemical and Computational Studies Using Silver Amalgam and HMDE Electrodes. Electrochimica Acta, 2014, 137, 564-574.	5.2	7
81	Antimicrobial effect of <i>Dinoponera quadriceps</i> (Hymenoptera: Formicidae) venom against <i>Staphylococcus aureus</i> strains. Journal of Applied Microbiology, 2014, 117, 390-396.	3.1	23
82	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
83	Resveratrol prevents social deficits in animal model of autism induced by valproic acid. Neuroscience Letters, 2014, 583, 176-181.	2.1	115
84	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
85	A comparative density functional theory study of electronic structure and optical properties of $\alpha$ -aminobutyric acid and its cocrystals with oxalic and benzoic acid. Chemical Physics Letters, 2013, 587, 20-24.	2.6	17
86	Assessing the Role of Water on the Electronic Structure and Vibrational Spectra of Monohydrated $\alpha$ -Aspartic Acid Crystals. Crystal Growth and Design, 2013, 13, 4844-4851.	3.0	22
87	An ab initio explanation of the activation and antagonism strength of an AMPA-sensitive glutamate receptor. RSC Advances, 2013, 3, 14988.	3.6	12
88	Quantum biochemistry study of the T3-785 tropocollagen triple-helical structure. Chemical Physics Letters, 2013, 559, 88-93.	2.6	31
89	Electrochemical and Monte Carlo studies of self-assembled trans-[Fe(cyclam)(NCS) <sub>2</sub> ] <sup>+</sup> complex ion on gold surface as electrochemical sensor for nitric oxide. Electrochimica Acta, 2013, 91, 1-10.	5.2	8
90	Immobilized invertase studies on glass-ceramic support from coal fly ashes. Chemical Engineering Journal, 2013, 214, 91-96.	12.7	13

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91	<sc>L</sc>-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
92	Dimethomorph electrooxidation: Analytical determination in grape-derived samples and mechanistic aspects. Electrochimica Acta, 2013, 107, 350-357.	5.2	10
93	Quantum analysis/improvement of antipsychotic's docking results. FASEB Journal, 2013, 27, 810.9.	0.5	0
94	Structural and optoelectronic properties, and infrared spectrum of cubic BaSnO <sub>3</sub> from first principles calculations. Journal of Applied Physics, 2012, 112, .	2.5	54
95	Four-level levodopa adsorption on C <sub>60</sub> fullerene for transdermal and oral administration: a computational study. RSC Advances, 2012, 2, 8306.	3.6	13
96	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
97	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
98	Electronic specific heat of an $\alpha$ -helical polypeptide and its biochemical variants. Chemical Physics Letters, 2012, 542, 123-127.	2.6	3
99	Explaining statin inhibition effectiveness of HMG-CoA reductase by quantum biochemistry computations. Physical Chemistry Chemical Physics, 2012, 14, 1389-1398.	2.8	61
100	Optical absorption and DFT calculations in $L$ -aspartic acid anhydrous crystals: Charge carrier effective masses point to semiconducting behavior. Physical Review B, 2012, 86, .	3.2	51
101	Direct electrochemical analysis of dexamethasone endocrine disruptor in raw natural waters. Journal of the Brazilian Chemical Society, 2012, 23, 110-119.	0.6	13
102	Performance of invertase immobilized on glass-ceramic supports in batch bioreactor. Chemical Engineering Journal, 2012, 187, 341-350.	12.7	8
103	Structural and electronic properties of Sr <sub>x</sub> Ba <sub>1-x</sub> SnO <sub>3</sub> from first principles calculations. Journal of Solid State Chemistry, 2012, 187, 186-194.	2.9	47
104	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
105	Quantum Biochemistry Description of the Human Dopamine D <sub>3</sub> Receptor in Complex with the Selective Antagonist Eticlopride. Journal of Proteomics and Bioinformatics, 2012, 05, .	0.4	15
106	Anhydrous crystals of DNA bases are wide gap semiconductors. Journal of Chemical Physics, 2011, 134, 175101.	3.0	45
107	Two-Level Adsorption of Ibuprofen on C <sub>60</sub> Fullerene for Transdermal Delivery: Classical Molecular Dynamics and Density Functional Theory Computations. Journal of Physical Chemistry C, 2011, 115, 24501-24511.	3.1	24
108	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



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109	Monoclinic and orthorhombic cysteine crystals are small gap insulators. Chemical Physics Letters, 2011, 512, 208-210.	2.6	19
110	Density functional theory study of the electronic properties of naphthofuranquinone compounds with antitrypanocidal activity. International Journal of Quantum Chemistry, 2011, 111, 1270-1279.	2.0	3
111	Structural, optoelectronic, infrared and Raman spectra of orthorhombic SrSnO <sub>3</sub> from DFT calculations. Journal of Solid State Chemistry, 2011, 184, 921-928.	2.9	85
112	Charge transport in fibrous/not fibrous $\alpha$ -helical and (5Q,7Q) $\alpha$ variant peptides. Applied Physics Letters, 2011, 98, .	3.3	10
113	Structural, electronic and optical properties of orthorhombic $\text{CdGeO}_3$ from first principles calculations. Journal of Solid State Chemistry, 2010, 183, 437-443.	2.9	7
114	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
115	Structural, electronic and optical properties of ilmenite and perovskite $\text{CdSnO}_3$ from DFT calculations. Journal of Physics Condensed Matter, 2010, 22, 435801.	1.8	20
116	$\text{CdXO}_3$ (X = C, Si, Ge, Sn, Pb) electronic band structures. Chemical Physics Letters, 2009, 480, 273-277.	2.6	20
117	Triclinic $\text{CdSiO}_3$ structural, electronic, and optical properties from first principles calculations. Journal Physics D: Applied Physics, 2009, 42, 155406.	2.8	22
118	Defects in Graphene-Based Twisted Nanoribbons: Structural, Electronic, and Optical Properties. Langmuir, 2009, 25, 4751-4759.	3.5	26
119	$\text{C}_{60}$ -derived nanobaskets: stability, vibrational signatures, and molecular trapping. Nanotechnology, 2009, 20, 395701.	2.6	8
120	The influence of 4-mercaptopyridine layer instability on rapid electron transfer reaction. Journal of Electroanalytical Chemistry, 2008, 619-620, 26-30.	3.8	6
121	Thermal effect on the dielectric function and small polaron hopping conduction in organic molecular crystals. Physics Letters, Section A: General, Atomic and Solid State Physics, 2008, 372, 3725-3728.	2.1	6
122	Band structure anisotropy effects on the ultrafast electron transport in 4H-SiC. Solid State Communications, 2008, 145, 397-400.	1.9	1
123	Möbius and twisted graphene nanoribbons: Stability, geometry, and electronic properties. Journal of Chemical Physics, 2008, 128, 164719.	3.0	54
124	Adsorption of Ascorbic Acid on the $\text{C}_{60}$ Fullerene. Journal of Physical Chemistry B, 2008, 112, 14267-14272.	2.6	30
125	First-principles calculations of structural, electronic and optical properties of orthorhombic $\text{CaPbO}_3$ . Journal Physics D: Applied Physics, 2008, 41, 065405.	2.8	10
126	Optical absorption and electronic band structure first-principles calculations of $\alpha$ -glycine crystals. Physical Review B, 2008, 77, .	3.2	37



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127	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
128	Correlation between Enterococcus faecalis Biofilms Development Stage and Quantitative Surface Roughness Using Atomic Force Microscopy. Microscopy and Microanalysis, 2008, 14, 150-158.	0.4	13
129	Si-SiO <sub>2</sub> -Si and Si-CaCO <sub>3</sub> -Si core-shell nanoparticles: Tuning light emission from infrared to ultraviolet. Journal of Applied Physics, 2007, 102, 023712.	2.5	0
130	CaO first-principles electronic properties and MOS device simulation. Journal Physics D: Applied Physics, 2007, 40, 1655-1658.	2.8	12
131	Transient transport in III-nitrides: interplay of momentum and energy relaxation times. Journal of Physics Condensed Matter, 2007, 19, 346214.	1.8	14
132	Two different incorporation sites of manganese in single-crystalline monohydrated L-asparagine studied by electron paramagnetic resonance. Physical Review B, 2007, 75, .	3.2	8
133	High lattice temperature effects on the ultrafast electron transport in 4H-SiC. Journal of Applied Physics, 2007, 102, 053710.	2.5	1
134	Consequences of nonstoichiometric SiO <sub>x</sub> interfacial layers on the electrical characterization of metal-oxide-semiconductor devices. Journal of Applied Physics, 2007, 101, 034509.	2.5	0
135	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. Journal Physics D: Applied Physics, 2007, 40, 5747-5752.	2.8	36
136	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
137	Hole-versus electron-based operations in SiGe nanocrystal nonvolatile memories. Applied Physics Letters, 2007, 90, 223504.	3.3	18
138	Structural, electronic, and optical absorption properties of orthorhombic CaSnO <sub>3</sub> through ab initio calculations. Journal of Physics Condensed Matter, 2007, 19, 106214.	1.8	29
139	First-principles calculations of structural, electronic, and optical absorption properties of CaCO <sub>3</sub> Vaterite. Chemical Physics Letters, 2007, 435, 59-64.	2.6	60
140	Dielectric function spectra from a nondegenerate polaron gas. Physics Letters, Section A: General, Atomic and Solid State Physics, 2007, 365, 478-482.	2.1	1
141	AFM and hydrodynamic electrochemical characterization of the self-assembled 1,4-dithiane on gold surface. Journal of Electroanalytical Chemistry, 2007, 603, 21-26.	3.8	6
142	Immobilization of urease on vapour phase stain etched porous silicon. Process Biochemistry, 2007, 42, 429-433.	3.7	25
143	Acoustic phonon transmission spectra in piezoelectric AlN/GaN Fibonacci phononic crystals. European Physical Journal B, 2007, 58, 379-387.	1.5	34
144	Influence of graded interfaces on the exciton energy of type-I and type-II Si/Si <sub>1-x</sub> Ge quantum wires. Journal of Materials Science, 2007, 42, 2314-2317.	3.7	5

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145	Production and characterization of the cashew ( <i>Anacardium occidentale</i> L.) peduncle bagasse ashes. <i>Journal of Food Engineering</i> , 2007, 79, 1432-1437.	5.2	44
146	Identification of lamivudine conformers by Raman scattering measurements and quantum chemical calculations. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , 2007, 43, 1885-1889.	2.8	14
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