

Paulo Cesar Piquini

List of Publications by Year in descending order

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2134
citing authors

#	ARTICLE	IF	CITATIONS
1	functional theory investigation of $\frac{3}{4}d$	1.1	211
2	Hydrogen Adsorption on Carbon-Doped Boron Nitride Nanotube. Journal of Physical Chemistry B, 2006, 110, 21184-21188.	1.2	105
3	Methylmercury's chemistry: From the environment to the mammalian brain. Biochimica Et Biophysica Acta - General Subjects, 2019, 1863, 129284.	1.1	78
4	Formation energy of native defects in BN nanotubes: an ab initio study. Nanotechnology, 2005, 16, 827-831.	1.3	74
5	Platinum-Based Nanoalloys Pt _n TM _{55-n} (TM = Co, Rh, Au): A Density Functional Theory Investigation. Journal of Physical Chemistry C, 2012, 116, 18432-18439.	1.5	65
6	Diameter dependence of mechanical, electronic, and structural properties of InAs and InP nanowires: A first-principles study. Physical Review B, 2010, 81, .	1.1	64
7	Ab initio study of native defects in SiC nanotubes. Physical Review B, 2006, 74, .	1.1	59
8	C-S cross-coupling of thiols with aryl iodides under ligand-free conditions using nano copper oxide as a recyclable catalyst in ionic liquid. Catalysis Science and Technology, 2011, 1, 569.	2.1	56
9	Band-Gap Design of Quaternary (In,Ga)(As,Sb) Semiconductors via the Inverse-Band-Structure Approach. Physical Review Letters, 2008, 100, 186403.	2.9	43
10	The role of electron localization in the atomic structure of transition-metal 13-atom clusters: the example of Co ₁₃ , Rh ₁₃ , and Hf ₁₃ . Physical Chemistry Chemical Physics, 2011, 13, 17242.	1.3	43
11	Electronic and structural trends in small GaAs clusters. Scripta Materialia, 1998, 10, 635-647.	0.5	36
12	Pseudopotential calculations of band gaps and band edges of short-period $\frac{1}{2}Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 307 Td$	1.1	35
13	Adsorption of NO on the Rh ₁₃ , Pd ₁₃ , Ir ₁₃ , and Pt ₁₃ Clusters: A Density Functional Theory Investigation. Journal of Physical Chemistry C, 2012, 116, 20540-20549.	1.5	33
14	Electronic properties of BN nanocones under electric fields. Microelectronics Journal, 2003, 34, 545-547.	1.1	32
15	The influence of the stacking orientation of C and BN stripes in the structure, energetics, and electronic properties of BC ₂ N nanotubes. Nanotechnology, 2011, 22, 205706.	1.3	31
16	Charge distributions in BN nanocones: electric field and tip termination effects. Chemical Physics Letters, 2004, 392, 428-432.	1.2	30
17	Theoretical studies of native defects in cubic boron nitride. Physical Review B, 1997, 56, 3556-3559.	1.1	28
18	Transition-metal 13-atom clusters assessed with solid and surface-biased functionals. Journal of Chemical Physics, 2011, 134, 134105.	1.2	27

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19	Synthesis of symmetric N,O-donor ligands derived from pyridoxal (vitamin B6): DFT studies and structural features of their binuclear chelate complexes with the oxophilic uranyl and vanadyl(V) cations. <i>Inorganica Chimica Acta</i> , 2014, 412, 6-14.	1.2	26
20	Revealing an unusual transparent phase of superhard iron tetraboride under high pressure. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2014, 111, 17050-17053.	3.3	23
21	On the contribution of electron transfer reactions to the quenching of tryptophan fluorescence. <i>Journal of Chemical Physics</i> , 1995, 103, 10614-10620.	1.2	22
22	Theoretical study of Si impurities in BN nanotubes. <i>European Physical Journal B</i> , 2004, 38, 515-518.	0.6	22
23	Diselenoamino acid derivatives as GPx mimics and as substrates of TrxR:in vitroandin silicostudies. <i>Organic and Biomolecular Chemistry</i> , 2018, 16, 3777-3787.	1.5	22
24	Synthesis and characterization of [Cd ₈ Cl ₂ Se(SePh) ₁₂ (PCy ₃) ₂] \cdot 2.5CH ₃ OH. <i>Journal of the Brazilian Chemical Society</i> , 2010, 21, 2146-2153.	0.6	19
25	Synthesis, crystal structure, and optical characteristics of [Pd ₂ Hg ₄ Cl ₆ {Te(DMB)} ₆] \cdot 2DMF, [HgClTe(DMB) ₄], and the ring-forming cluster [Pd ₁₂ (TePh) ₂₄] \cdot 2DMF. <i>New Journal of Chemistry</i> , 2014, 38, 2394-2399.	1.4	19
26	SOD activity of new copper II complexes with ligands derived from pyridoxal and toxicity in <i>Caenorhabditis elegans</i> . <i>Journal of Inorganic Biochemistry</i> , 2020, 204, 110950.	1.5	19
27	Theoretical investigation on the stability and properties of a (10,0) BN ϵ -AlN nanotube junction. <i>Nanotechnology</i> , 2006, 17, 1637-1641.	1.3	18
28	AlN, GaN, Al Ga \hat{a} N nanotubes and GaN/Al Ga \hat{a} N nanotube heterojunctions. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2010, 374, 877-881.	0.9	18
29	Synthesis and structure of [ReOSe(2-Se-py) ₃]: A rhenium(V) complex with selenium(0) as a ligand. <i>Inorganic Chemistry Communication</i> , 2014, 45, 48-50.	1.8	18
30	Theoretical investigation of TiB ₂ nanotubes. <i>Microelectronics Journal</i> , 2003, 34, 495-497.	1.1	17
31	Lithium-functionalized boron phosphide nanotubes (BPNTs) as an efficient hydrogen storage carrier. <i>International Journal of Hydrogen Energy</i> , 2021, 46, 20586-20593.	3.8	17
32	Synthesis, structure and SOD activity of Mn complexes with symmetric Schiff base ligands derived from pyridoxal. <i>Polyhedron</i> , 2015, 102, 176-184.	1.0	16
33	Oxazolidine copper complexes: Synthesis, characterization and superoxide dismutase activity of copper(II) complexes with oxazolidine ligands derived from hydroxyquinoline carboxaldehyde. <i>Applied Organometallic Chemistry</i> , 2018, 32, e4218.	1.7	16
34	Electronic properties of selected BN nanocones. <i>Materials Characterization</i> , 2003, 50, 179-182.	1.9	15
35	Photophysical and photocatalytic properties of cororophyll and chlorophyll. <i>Computational Materials Science</i> , 2019, 158, 228-234.	1.4	15
36	Electronic and structural properties of InAs/InP core/shell nanowires: A first principles study. <i>Journal of Applied Physics</i> , 2012, 111, 054315.	1.1	14

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37	First-principles study of HgTe/CdTe heterostructures under perturbations preserving time-reversal symmetry. <i>Physical Review B</i> , 2014, 90, .	1.1	14
38	New oxidovanadium(V) complexes of the cation [VO]3+: Synthesis, structural characterization and DFT studies. <i>Polyhedron</i> , 2012, 36, 21-29.	1.0	13
39	Synthesis, characterization and phosphatase inhibitory activity of dioxidovanadium(V) complexes with Schiff base ligands derived from pyridoxal and resorcinol. <i>Polyhedron</i> , 2017, 130, 184-194.	1.0	13
40	The influence of the tip structure and the electric field on BN nanocones. <i>Nanotechnology</i> , 2005, 16, 302-306.	1.3	12
41	Pt, Pd and Hg Complexes with Potentially Tridentate Telluroether Ligands. <i>European Journal of Inorganic Chemistry</i> , 2015, 2015, 3748-3757.	1.0	12
42	Defect complexes in GaAs: First-principles calculations. <i>Physical Review B</i> , 1997, 56, 13073-13076.	1.1	11
43	Energetics and electronic properties of BN nanocones with pentagonal rings at their apexes. <i>European Physical Journal D</i> , 2003, 23, 91-93.	0.6	11
44	First principles study of vacancies and Al substitutional impurities in δ -TiN. <i>Thin Solid Films</i> , 2006, 515, 2730-2733.	0.8	11
45	Energetic and electronic properties of BN nanotube bundle under pressure. <i>Physica Status Solidi (B): Basic Research</i> , 2007, 244, 110-115.	0.7	11
46	On the p-type character of Cd-and Zn-doped InAs nanowires. <i>Nanotechnology</i> , 2011, 22, 265203.	1.3	11
47	Structural, electronic, and vibrational properties of B_xN_y ($x + y = 6$) clusters. <i>International Journal of Quantum Chemistry</i> , 2003, 95, 329-335.	1.0	10
48	Tchnetium complexes with arylselenolato and aryltelluroolato ligands. <i>Dalton Transactions</i> , 2017, 46, 9280-9286.	1.6	10
49	Corrole Fullerenes Dyads: Stability, Photophysical, and Redox Properties. <i>Journal of Physical Chemistry C</i> , 2019, 123, 20869-20876.	1.5	10
50	HfS ₂ and TiS ₂ Monolayers with Adsorbed C, N, P Atoms: A First Principles Study. <i>Catalysts</i> , 2020, 10, 94.	1.6	10
51	From Monolayers to Nanotubes: Toward Catalytic Transition-Metal Dichalcogenides for Hydrogen Evolution Reaction. <i>Energy & Fuels</i> , 2021, 35, 6282-6288.	2.5	10
52	Unveiling the photophysical, biomolecule binding and photo-oxidative capacity of novel Ru(II)-polypyridyl corroles: A multipronged approach. <i>Journal of Molecular Liquids</i> , 2021, 340, 117223.	2.3	10
53	Studies of the local reactivity of surfaces using chemical based principles. <i>Surface Science</i> , 1994, 313, 41-51.	0.8	9
54	Low hole effective mass in thin InAs nanowires. <i>Applied Physics Letters</i> , 2010, 96, .	1.5	9

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55	High pressure driven superconducting critical temperature tuning in Sb ₂ Se ₃ topological insulator. Applied Physics Letters, 2016, 108, 212601.	1.5	9
56	Tunable interaction between metal clusters and graphene. Physical Chemistry Chemical Physics, 2017, 19, 22153-22160.	1.3	8
57	Symmetrical and Unsymmetrical 4,7-Bis(arylvinyloxy)benzo[1,3-d]chalcogenodiazoles: Synthesis, Photophysical and Electrochemical Properties and Biomolecular Interaction Studies. European Journal of Organic Chemistry, 2020, 2020, 348-361.	1.2	8
58	Building Hg(II)/Cu(I) multinuclear compounds from mercury bis(phenylselenolate). Journal of Organometallic Chemistry, 2012, 703, 9-15.	0.8	7
59	Synthesis and characterisation of [Cu ₄ In(PPH) ₃ SePh ₃ (¹ / ₄ -SePh) ₃ (¹ / ₄ -SePh) ₃], ₇ and its application as a precursor of a sensitizer for a photocatalyst. New Journal of Chemistry, 2019, 43, 14196-14201.	1.4	7
60	Oxidation of crude palladium powder by a diiodine adduct of (2-PyTe) ₂ to obtain the novel PdII complex [Pd(TePy-2)(I ₂ TePy-2)]. Inorganic Chemistry Communication, 2020, 118, 107966.	1.8	7
61	First-principles study of the hBN(0001)/cBN(111) interface. Physical Review B, 2005, 71, .	1.1	6
62	The effects of an explicit water environment on the interaction of a single wall carbon nanotube with amino acids: A theoretical study. Chemical Physics Letters, 2011, 518, 81-86.	1.2	6
63	Synthesis, X-ray structural features, DFT calculations and fluorescence studies of a new pyridoxal-benzimidazole ligand and its respective molybdenum complex. New Journal of Chemistry, 2014, 38, 3092-3101.	1.4	6
64	New manganese(II) and nickel(II) coordination compounds with N,O-polydentate ligands obtained from pyridoxal and tripodal units. Journal of Molecular Structure, 2016, 1120, 163-170.	1.8	6
65	Peroxidase activity of new mixed-valence cobalt complexes with ligands derived from pyridoxal. Applied Organometallic Chemistry, 2019, 33, e4903.	1.7	6
66	Synthesis and characterization of aryltellurium compounds including mixed-valence derivatives: Evaluation of Te ^{IV} -S, Te ^{IV} -X and X ^{IV} -X (X=Br, I) interactions. Journal of Organometallic Chemistry, 2020, 929, 121553.	0.8	6
67	Ab initio self-consistent-field studies of the structure, energetics and bonding of small gallium arsenide clusters. Zeitschrift für Physik D-Atoms Molecules and Clusters, 1995, 33, 125-131.	1.0	5
68	Theoretical investigation of the hBN(0001)/cBN(111) interface. Diamond and Related Materials, 2008, 17, 1963-1968.	1.8	5
69	Using superlattice ordering to reduce the band gap of random (In,Ga)As/InP alloys to a target value via the inverse band structure approach. Physical Review B, 2008, 78, .	1.1	5
70	Concerted-exchange mechanism for antistructure pair defects in GaAs. Solid State Communications, 1999, 110, 457-461.	0.9	4
71	Ab initio study of BN nanoarches' surfaces. Surface Science, 2004, 555, 179-186.	0.8	4
72	Theoretical investigation of BN armchair and zigzag nanoarch surfaces. Nanotechnology, 2006, 17, 556-560.	1.3	4

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73	Synthesis, structural and optical studies of several new ditelluroether iodides. <i>Polyhedron</i> , 2012, 39, 106-112.	1.0	4
74	Asymmetric and symmetric triazenido cyclopalladated complexes: Synthesis, structural analysis and DFT calculations. <i>Journal of Molecular Structure</i> , 2015, 1083, 311-318.	1.8	4
75	Photophysics of Donor/Acceptor Functionalized Corroles: a First-Principles Study. <i>Brazilian Journal of Physics</i> , 2019, 49, 502-507.	0.7	4
76	Intermolecular metallophilic interactions in palladium(II) chalcogenolate compounds – An experimental and theoretical study. <i>Polyhedron</i> , 2020, 177, 114315.	1.0	4
77	Structural and electronic studies of Ga ₃ As ₃ , Ga ₄ As ₃ , and Ga ₃ As ₄ . <i>International Journal of Quantum Chemistry</i> , 1994, 52, 571-577.	1.0	3
78	Alloying InAs and InP nanowires for optoelectronic applications: A first principles study. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2014, 378, 2872-2875.	0.9	3
79	Oxidation of InP nanowires: a first principles molecular dynamics study. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 31101-31106.	1.3	3
80	Excited-state investigations of meso-mono-substituted-(amino-ferrocenyl)porphyrins: Experimental and theoretical approaches. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2019, 384, 112048.	2.0	3
81	Band folding, strain, confinement, and surface relaxation effects on the electronic structure of GaAs and GaP: from bulk to nanowires. <i>European Physical Journal B</i> , 2019, 92, 1.	0.6	3
82	Mn-doped cubic BN as an atomiclike memory device: A density functional study. <i>Physical Review B</i> , 2010, 81, .	1.1	2
83	One-pot™ synthesis and redox evaluations of chiral chalcogenocysteinol and β^2 -bis-chalcogenoamine derivatives from <i>l</i> -serine methyl ester. <i>New Journal of Chemistry</i> , 2017, 41, 7424-7431.	1.4	2
84	Theoretical investigation of the anchoring and activity of a gold cluster on two-dimensional substrates. <i>Materials Research Express</i> , 2019, 6, 075069.	0.8	2
85	Organically templated zinc selenite compounds: synthesis, structural chemistry and DFT calculations. <i>New Journal of Chemistry</i> , 2020, 44, 6699-6703.	1.4	2
86	Large Telluroxane Bowls Connected by a Layer of Iodine Ions. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 15517-15523.	7.2	2
87	Theoretical study of defect complexes related with antisites in GaAs. <i>Radiation Effects and Defects in Solids</i> , 1998, 146, 65-70.	0.4	1
88	Large Telluroxane Bowls Connected by a Layer of Iodine Ions. <i>Angewandte Chemie</i> , 2021, 133, 15645-15651.	1.6	1
89	Using topological analysis of the electron density to study a geometry-electronic structure relationship in M (d ⁵ –10)–O and E–O (E=As,Te) compounds. <i>Computational and Theoretical Chemistry</i> , 2021, 1201, 113279.	1.1	1
90	Electronic and structural properties of two mirrored boron-nitride nanocones with 240° disclination. <i>Brazilian Journal of Physics</i> , 2009, 39, 239-241.	0.7	1

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91	Synthesis and structural characterization of two exotic examples of aryltelluroate cluster compounds: $[Ag_4Hg(\mu\text{-Te Py-}^i\text{Te})_3(\mu_3\text{-Te Py-}^i\text{Te})_2(\mu_3\text{-Te Py-}^i\text{N,Te})(PPh_3)_2]$ and $[Cu(\text{phen})]_3(\mu_3\text{-TePh})_3(\text{CuCl}) \cdot 0.5C_2H_6O$. <i>Inorganic Chemistry Communication</i> , 2021, , 109024.	1.8	1
92	Electronic and structural properties of defects in c-BN. <i>International Journal of Quantum Chemistry</i> , 1997, 65, 941-946.	1.0	0
93	Theoretical investigation of the HgTe topological edge states with a Fe impurity. <i>Physica B: Condensed Matter</i> , 2022, 630, 413673.	1.3	0