Paulo Cesar Piquini

List of Publications by Year
in descending order

93 papers	1,738 citations	331538 21 h-index	330025 37 g-index
94 all docs	94 docs citations	94 times ranked	2134 citing authors

#	Article	IF	Citations
1	Theoretical investigation of the HgTe topological edge states with a Fe impurity. Physica B: Condensed Matter, 2022, 630, 413673.	1.3	0
2	From Monolayers to Nanotubes: Toward Catalytic Transition-Metal Dichalcogenides for Hydrogen Evolution Reaction. Energy & Fuels, 2021, 35, 6282-6288.	2.5	10
3	Large Telluroxane Bowls Connected by a Layer of Iodine Ions. Angewandte Chemie, 2021, 133, 15645-15651.	1.6	1
4	Large Telluroxane Bowls Connected by a Layer of Iodine Ions. Angewandte Chemie - International Edition, 2021, 60, 15517-15523.	7.2	2
5	Lithium-functionalized boron phosphide nanotubes (BPNTs) as an efficient hydrogen storage carrier. International Journal of Hydrogen Energy, 2021, 46, 20586-20593.	3.8	17
6	Using topological analysis of the electron density to study a geometry-electronic structure relationship in M (d5â€“10)â€¦O and Eâ€¦O (EÂ=ÂSe,Te) compounds. Computational and Theoretical Chemistry, 2021, 1201, 113279.	1.1	1
7	Unveiling the photophysical, biomolecule binding and photo-oxidative capacity of novel Ru(II)-polypyridyl corroles: A multipronged approach. Journal of Molecular Liquids, 2021, 340, 117223.	2.3	10
8	Synthesis and structural characterization of two exotic examples of aryltellurolate cluster compounds: [Ag4Hg(Âµ-Te Py-Î²Te)3(Âµ3-Te Py-Î²Te)2(Âµ3-Te Py-Î²N,Te)(PPh3)2] and [{Cu(phen)}3(Âµ3-TePh)3(CuCl)]â‹…0.5C2H6O. Inorganic Chemistry Communication, 2021, , 109024.	1.8	1
9	Intermolecular metallophilic interactions in palladium(II) chalcogenolate compounds â€“ An experimental and theoretical study. Polyhedron, 2020, 177, 114315.	1.0	4
10	Symmetrical and Unsymmetrical 4,7â€Bisâ€arylvinylâ€benzoâ€2,1,3â€chalcogenodiazoles: Synthesis, Photophysical and Electrochemical Properties and Biomolecular Interaction Studies. European Journal of Organic Chemistry, 2020, 2020, 348-361.	1.2	8
11	SOD activity of new copper II complexes with ligands derived from pyridoxal and toxicity in Caenorhabditis elegans. Journal of Inorganic Biochemistry, 2020, 204, 110950.	1.5	19
12	Synthesis and characterization of aryltellurium compounds including mixed-valence derivativesÂâˆ’Âevaluation of Teâ‹…â‹…â‹…S, Teâ‹…â‹…â‹…X and Xâ‹…â‹…â‹…X (XÂ=ÂBr, I) interactions. Journal of Organometallic Chem 2020, 929, 121553.	0.8	6
13	Oxidation of crude palladium powder by a diiodine adduct of (2-PyTe)2 to obtain the novel PdII complex [PdI(TePy-2)(I2TePy-2)2]. Inorganic Chemistry Communication, 2020, 118, 107966.	1.8	7
14	HfS2 and TiS2 Monolayers with Adsorbed C, N, P Atoms: A First Principles Study. Catalysts, 2020, 10, 94.	1.6	10
15	Organically templated zinc selenite compounds: synthesis, structural chemistry and DFT calculations. New Journal of Chemistry, 2020, 44, 6699-6703.	1.4	2
16	Synthesis and characterisation of [Cu₄In(PPh₃)₃SePh(Î¼-SePh)₃(Î¼₃-SePh)₃], and its application as a precursor of a sensitizer for a photocatalyst. New Journal of Chemistry, 2019, 43, 14196-14201.	1.4	7
17	Corroleâ€“Fullerene Dyads: Stability, Photophysical, and Redox Properties. Journal of Physical Chemistry C, 2019, 123, 20869-20876.	1.5	10
18	Excited-state investigations of meso-mono-substituted-(amino-ferrocenyl)porphyrins: Experimental and theoretical approaches. Journal of Photochemistry and Photobiology A: Chemistry, 2019, 384, 112048.	2.0	3

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19	Band folding, strain, confinement, and surface relaxation effects on the electronic structure of GaAs and GaP: from bulk to nanowires. European Physical Journal B, 2019, 92, 1.	0.6	3
20	Methylmercury's chemistry: From the environment to the mammalian brain. Biochimica Et Biophysica Acta - General Subjects, 2019, 1863, 129284.	1.1	78
21	Peroxidase activity of new mixedâ€valence cobalt complexes with ligands derived from pyridoxal. Applied Organometallic Chemistry, 2019, 33, e4903.	1.7	6
22	Theoretical investigation of the anchoring and activity of a gold cluster on two-dimensional substrates. Materials Research Express, 2019, 6, 075069.	0.8	2
23	Photophysics of Donor/Acceptor Functionalized Corroles: a First-Principles Study. Brazilian Journal of Physics, 2019, 49, 502-507.	0.7	4
24	Photophysical and photocatalytic properties of corrophyll and chlorophyll. Computational Materials Science, 2019, 158, 228-234.	1.4	15
25	Oxazolidine copper complexes: Synthesis, characterization and superoxide dismutase activity of copper(II) complexes with oxazolidine ligands derived from hydroxyquinoline carboxaldehyde. Applied Organometallic Chemistry, 2018, 32, e4218.	1.7	16
26	Diselenoamino acid derivatives as GPx mimics and as substrates of TrxR:in vitroandin silicostudies. Organic and Biomolecular Chemistry, 2018, 16, 3777-3787.	1.5	22
27	Synthesis, characterization and phosphatase inhibitory activity of dioxidovanadium(V) complexes with Schiff base ligands derived from pyridoxal and resorcinol. Polyhedron, 2017, 130, 184-194.	1.0	13
28	Technetium complexes with arylselenolato and aryltellurolato ligands. Dalton Transactions, 2017, 46, 9280-9286.	1.6	10
29	â€˜One-potâ€™ synthesis and redox evaluations of chiral chalcogenocysteinol and Î²-bis-chalcogenoamine derivatives from <scp>l</scp>-serine methyl ester. New Journal of Chemistry, 2017, 41, 7424-7431.	1.4	2
30	Tunable interaction between metal clusters and graphene. Physical Chemistry Chemical Physics, 2017, 19, 22153-22160.	1.3	8
31	High pressure driven superconducting critical temperature tuning in Sb2Se3 topological insulator. Applied Physics Letters, 2016, 108, 212601.	1.5	9
32	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
33	Oxidation of InP nanowires: a first principles molecular dynamics study. Physical Chemistry Chemical Physics, 2016, 18, 31101-31106.	1.3	3
34	Pt, Pd and Hg Complexes with Potentially Tridentate Telluroether Ligands. European Journal of Inorganic Chemistry, 2015, 2015, 3748-3757.	1.0	12
35	Asymmetric and symmetric triazenido cyclopalladated complexes: Synthesis, structural analysis and DFT calculations. Journal of Molecular Structure, 2015, 1083, 311-318.	1.8	4
36	Synthesis, structure and SOD activity of Mn complexes with symmetric Schiff base ligands derived from pyridoxal. Polyhedron, 2015, 102, 176-184.	1.0	16

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37	First-principles study of HgTe/CdTe heterostructures under perturbations preserving time-reversal symmetry. Physical Review B, 2014, 90, .	1.1	14
38	Revealing an unusual transparent phase of superhard iron tetraboride under high pressure. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 17050-17053.	3.3	23
39	Synthesis and structure of [ReOSe(2-Se-py)3]: A rhenium(V) complex with selenium(0) as a ligand. Inorganic Chemistry Communication, 2014, 45, 48-50.	1.8	18
40	Synthesis of symmetric N,O-donor ligands derived from pyridoxal (vitamin B6): DFT studies and structural features of their binuclear chelate complexes with the oxofilic uranyl and vanadyl(V) cations. Inorganica Chimica Acta, 2014, 412, 6-14.	1.2	26
41	Synthesis, crystal structure, and optical characteristics of [Pd₂Hg₄Cl₆{Te(DMB)}₆]Â·2DMF, [HgClTe(DMB)]₄, and the ring-forming cluster [Pd₁₂(TePh)₂₄]Â·2DMF. New Journal of Chemistry, 2014, 38, 2394-2399.	1.4	19
42	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
43	Alloying InAs and InP nanowires for optoelectronic applications: A first principles study. Physics Letters, Section A: General, Atomic and Solid State Physics, 2014, 378, 2872-2875.	0.9	3
44	Building Hg(II)/Cu(I) multinuclear compounds from mercury bis(phenylselenolate). Journal of Organometallic Chemistry, 2012, 703, 9-15.	0.8	7
45	Adsorption of NO on the Rh₁₃, Pd₁₃, Ir₁₃, and Pt₁₃ Clusters: A Density Functional Theory Investigation. Journal of Physical Chemistry C, 2012, 116, 20540-20549.	1.5	33
46	Platinum-Based Nanoalloys Pt_nTM_{55â€“n} (TM = Co, Rh, Au): A Density Functional Theory Investigation. Journal of Physical Chemistry C, 2012, 116, 18432-18439.	1.5	65
47	Electronic and structural properties of InAs/InP core/shell nanowires: A first principles study. Journal of Applied Physics, 2012, 111, 054315.	1.1	14
48	New oxidovanadium(V) complexes of the cation [VO]3+: Synthesis, structural characterization and DFT studies. Polyhedron, 2012, 36, 21-29.	1.0	13
49	Synthesis, structural and optical studies of several new ditelluroether iodides. Polyhedron, 2012, 39, 106-112.	1.0	4
50	Transition-metal 13-atom clusters assessed with solid and surface-biased functionals. Journal of Chemical Physics, 2011, 134, 134105.	1.2	27
51	The role of electron localization in the atomic structure of transition-metal 13-atom clusters: the example of Co13, Rh13, and Hf13. Physical Chemistry Chemical Physics, 2011, 13, 17242.	1.3	43
52	Câ€“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
53	The influence of the stacking orientation of C and BN stripes in the structure, energetics, and electronic properties of BC₂N nanotubes. Nanotechnology, 2011, 22, 205706.	1.3	31
54	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

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55	On the p-type character of Cd-and Zn-doped InAs nanowires. Nanotechnology, 2011, 22, 265203.	1.3	11
56	AlN, GaN, Al Ga1â˜'N nanotubes and GaN/Al Ga1â˜'N nanotube heterojunctions. Physics Letters, Section A: General, Atomic and Solid State Physics, 2010, 374, 877-881.	0.9	18
57	Synthesis and characterization of [Cd8Cl2Se(SePh)12(PCy3)2]Â·2.5CH3OH. Journal of the Brazilian Chemical Society, 2010, 21, 2146-2153.	0.6	19
58	Mn-doped cubic BN as an atomiclike memory device: A density functional study. Physical Review B, 2010, 81, .	1.1	2
59	Low hole effective mass in thin InAs nanowires. Applied Physics Letters, 2010, 96, .	1.5	9
60	Density functional theory investigation of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mn>3</mml:mn><mml:mi>d</mml:mi></mml:mrow></mml:math>,<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mn>4</mml:mn><mml:mi>d</mml:mi></mml:mrow></mml:math>, and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:	1.1	211
61	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
62	Electronic and structural properties of two mirrored boron-nitride nanocones with 240Âº disclination. Brazilian Journal of Physics, 2009, 39, 239-241.	0.7	1
63	Theoretical investigation of the hBN(0001)/cBN(111) interface. Diamond and Related Materials, 2008, 17, 1963-1968.	1.8	5
64	Pseudopotential calculations of band gaps and band edges of short-period<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mo>(</mml:mo><mml:mi) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 387 Td (	1.1	35
65	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
66	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
67	Energetic and electronic properties of BN nanotube bundle under pressure. Physica Status Solidi (B): Basic Research, 2007, 244, 110-115.	0.7	11
68	Hydrogen Adsorption on Carbon-Doped Boron Nitride Nanotube. Journal of Physical Chemistry B, 2006, 110, 21184-21188.	1.2	105
69	Ab initiostudy of native defects in SiC nanotubes. Physical Review B, 2006, 74, .	1.1	59
70	First principles study of vacancies and Al substitutional impurities in Î´-TiN. Thin Solid Films, 2006, 515, 2730-2733.	0.8	11
71	Theoretical investigation of BN armchair and zigzag nanoarch surfaces. Nanotechnology, 2006, 17, 556-560.	1.3	4
72	Theoretical investigation on the stability and properties of a (10,0) BNâ€“AlN nanotube junction. Nanotechnology, 2006, 17, 1637-1641.	1.3	18

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73	First-principles study of the(112Â¯0)hBNâˆ•(112Â¯)cBNinterface. Physical Review B, 2005, 71, .	1.1	6
74	The influence of the tip structure and the electric field on BN nanocones. Nanotechnology, 2005, 16, 302-306.	1.3	12
75	Formation energy of native defects in BN nanotubes: anab initiostudy. Nanotechnology, 2005, 16, 827-831.	1.3	74
76	Theoretical study of Si impurities in BN nanotubes. European Physical Journal B, 2004, 38, 515-518.	0.6	22
77	Ab initio study of BN nanoarches' surfaces. Surface Science, 2004, 555, 179-186.	0.8	4
78	Charge distributions in BN nanocones: electric field and tip termination effects. Chemical Physics Letters, 2004, 392, 428-432.	1.2	30
79	Energetics and electronic properties of BN nanocones with pentagonal rings at their apexes. European Physical Journal D, 2003, 23, 91-93.	0.6	11
80	Electronic properties of selected BN nanocones. Materials Characterization, 2003, 50, 179-182.	1.9	15
81	Electronic properties of BN nanocones under electric fields. Microelectronics Journal, 2003, 34, 545-547.	1.1	32
82	Theoretical investigation of TiB2 nanotubes. Microelectronics Journal, 2003, 34, 495-497.	1.1	17
83	Structural, electronic, and vibrational properties of BxNy (x +y = 6) clusters. International Journal of Quantum Chemistry, 2003, 95, 329-335.	1.0	10
84	Concerted-exchange mechanism for antistructure pair defects in GaAs. Solid State Communications, 1999, 110, 457-461.	0.9	4
85	Electronic and structural trends in small GaAs clusters. Scripta Materialia, 1998, 10, 635-647.	0.5	36
86	Theoretical study of defect complexes related with antisites in GaAs. Radiation Effects and Defects in Solids, 1998, 146, 65-70.	0.4	1
87	Theoretical studies of native defects in cubic boron nitride. Physical Review B, 1997, 56, 3556-3559.	1.1	28
88	Defect complexes in GaAs:â€ƒFirst-principles calculations. Physical Review B, 1997, 56, 13073-13076.	1.1	11
89	Electronic and structural properties of defects in c-BN. International Journal of Quantum Chemistry, 1997, 65, 941-946.	1.0	0
90	Ab initio self-consistent-field studies of the structure, energetics and bonding of small gallium arsenide clusters. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1995, 33, 125-131.	1.0	5

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91	On the contribution of electron transfer reactions to the quenching of tryptophan fluorescence. Journal of Chemical Physics, 1995, 103, 10614-10620.	1.2	22
92	Structural and electronic studies of Ga3As3, Ga4As3, and Ga3As4. International Journal of Quantum Chemistry, 1994, 52, 571-577.	1.0	3
93	Studies of the local reactivity of surfaces using chemical based principles. Surface Science, 1994, 313, 41-51.	0.8	9