Penny P Govender

List of Publications by Year
in descending order

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84	2,235	279487 23	243296 44
papers	citations	h-index	g-index

85	85	85	3168
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Atomistic insight into the significantly enhanced photovoltaic cells of monolayer GaTe₂ via two-dimensional van der Waals heterostructures engineering. ChemistrySelect, 2022, 7, 629-644.	0.7	0
2	Imidazolium-Quaternized Poly(2,6-Dimethyl-1,4-Phenylene Oxide)/Zeolitic Imidazole Framework-8 Composite Membrane as Polymer Electrolyte for Fuel-Cell Application. Polymers, 2022, 14, 595.	2.0	5
3	Electrochemical Detection of Tetracycline on Highly Sensitive Benzene Sourced CVD Grapheneâ€Gold Nanoparticles Nanointerfaces. Electroanalysis, 2021, 33, 412-420.	1.5	16
4	Exploring the Optical, Structural and Electronic Properties of a Two-Dimensional GaSe/C2N van der Waals Heterostructure As a Photovoltaic Cell: A Computational Investigation. Journal of Electronic Materials, 2021, 50, 620-628.	1.0	5
5	Remarkable Enhancement of Euâ€“TiO2â€“GO Composite for Photodegradation of Indigo Carmine: A Design Method Based on Computational and Experimental Perspectives. Catalysis Letters, 2021, 151, 1111-1126.	1.4	14
6	Prospective of functionalized nanomaterials in environmental science: A nanotechnological approach. , 2021, , 13-60.		1
7	Electro-catalytic amplified sensor for determination of N-acetylcysteine in the presence of theophylline confirmed by experimental coupled theoretical investigation. Scientific Reports, 2021, 11, 1006.	1.6	4
8	Electrochemical detection of amoxicillin on 2D graphene-gold nanoparticle-Lacasse bio-interfaces: Combined experimental and theoretical study. Chemical Physics Letters, 2021, 764, 138278.	1.2	12
9	Insights into the complementary behaviour of Gd doping in GO/Gd/ZnO composites as an efficient candidate towards photocatalytic degradation of indigo carmine dye. Journal of Materials Science, 2021, 56, 8511-8527.	1.7	16
10	MoS₂ Nanosheet/ZnS Composites for the Visible-Light-Assisted Photocatalytic Degradation of Oxytetracycline. ACS Applied Nano Materials, 2021, 4, 4721-4734.	2.4	61
11	SF6 decomposed gas sensing performance of van der Waals layered cobalt oxyhydroxide: insights from a computational study. Journal of Molecular Modeling, 2021, 27, 158.	0.8	0
12	Developing a simple boxâ€“behnken experimental design on the removal of doxorubicin anticancer drug using Fe3O4/graphene nanoribbons adsorbent. Environmental Research, 2021, 200, 111522.	3.7	29
13	Tuning the aqueous solubility, chemical reactivity and absorption wavelength of azo dye through systematic adjustment of molecular charge density: a DFT study. Molecular Physics, 2020, 118, .	0.8	4
14	In vitro and in silico studies of the antifungal properties of the bulb and leaves extracts of Drimia delagoensis Baker (Jessop). Advances in Traditional Medicine, 2020, 20, 373-379.	1.0	2
15	The role of magnetite/graphene oxide nano-composite as a high-efficiency adsorbent for removal of phenazopyridine residues from water samples, an experimental/theoretical investigation. Journal of Molecular Liquids, 2020, 298, 112040.	2.3	319
16	Computational investigation of the binding characteristics of Î²-amyloid fibrils. Biophysical Chemistry, 2020, 256, 106281.	1.5	10
17	Ligand-based pharmacophore modelling and virtual screening for the identification of amyloid-beta diagnostic molecules. Journal of Molecular Graphics and Modelling, 2020, 101, 107711.	1.3	12
18	Computational screening of vdWs heterostructures of BSe with MoSe2 and WSe2 as sustainable hydrogen production materials. Current Applied Physics, 2020, , .	1.1	1

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19	Composite 2D Nanointerfaces for Electrochemical Biosensing: An Experimental and Theoretical Study. ACS Applied Bio Materials, 2020, 3, 8676-8687.	2.3	3
20	Thermoelectric, Electronic, and Optical Response of Nanostructured Alâ€doped ZnO @ 2Dâ€TiC Composite. ChemistrySelect, 2020, 5, 13144-13154.	0.7	5
21	Twoâ€dimensional CoOOH as a Highly Sensitive and Selective H₂S, HCN and HF Gas Sensor: A Computational Investigation. Electroanalysis, 2020, 32, 2764-2774.	1.5	8
22	Adsorption behaviour of Si anchored on g-C3N4/graphene van der Waals heterostructure for selective sensing of toxic gases: Insights from a first-principles study. Applied Surface Science, 2020, 525, 146590.	3.1	24
23	Tuning the electronic, optical and structural properties of GaS/C2N van der Waals heterostructure for photovoltaic application: first-principle calculations. SN Applied Sciences, 2020, 2, 1.	1.5	16
24	Switchable Graphene-Based Bioelectronics Interfaces. Chemosensors, 2020, 8, 45.	1.8	14
25	Highly Selective and Sensitive Detection of Formaldehyde by Î²₁₂-Borophene/SnO₂ Heterostructures: The Role of an External Electric Field and In-Plain Biaxial Strain. Journal of Physical Chemistry A, 2020, 124, 2288-2300.	1.1	29
26	Electrochemical anticancer drug sensor for determination of raloxifene in the presence of tamoxifen using graphene-CuO-polypyrrole nanocomposite structure modified pencil graphite electrode: Theoretical and experimental investigation. Journal of Molecular Liquids, 2020, 311, 113314.	2.3	24
27	One-step synthesized 2D heteroatom doped graphene for high throughput electrochemical biosensing: A combined experimental and computational studies. Diamond and Related Materials, 2019, 100, 107592.	1.8	10
28	Prediction of aqueous solubility by treatment of COSMO-RS data with empirical solubility equations: the roles of global orbital cut-off and COSMO solvent radius. Theoretical Chemistry Accounts, 2019, 138, 1.	0.5	9
29	Experimental and Computational Design of Highly Active Ceâ€“ZrO2â€“GO Photocatalyst for Eosin Yellow Dye Degradation: The Role of Interface and Ce3+ Ion. Catalysis Letters, 2019, 149, 1633-1650.	1.4	18
30	High-Throughput 2D Heteroatom Graphene Bioelectronic Nanosculpture: A Combined Experimental and Theoretical Study. ACS Applied Materials & Interfaces, 2019, 11, 11238-11250.	4.0	5
31	A theoretical study of 2D AlN on 3D C4H6N6Ni2 clathrate thermoelectric material composites. SN Applied Sciences, 2019, 1, 1.	1.5	1
32	Evaluating Iso-Mukaadial Acetate and Ursolic Acid Acetate as Plasmodium falciparum Hypoxanthine-Guanine-Xanthine Phosphoribosyltransferase Inhibitors. Biomolecules, 2019, 9, 861.	1.8	13
33	Tuning the electronic properties and interfacial interactions of WS2/ZrO2(001) heterostructures by an external electric field, interlayer coupling and monolayer to fewâ€layer of WS2 sheets. Materials Chemistry and Physics, 2019, 224, 107-116.	2.0	9
34	Hierarchically assembled two-dimensional gold boron nitride-tungsten disulphide nanohybrid interface system for electrobiocatalytic applications. Materials Chemistry and Physics, 2019, 226, 129-140.	2.0	9
35	Tuning the electronic and structural properties of Gd-TiO2-GO nanocomposites for enhancing photodegradation of IC dye: The role of Gd3+ ion. Applied Catalysis B: Environmental, 2019, 243, 106-120.	10.8	60
36	The effects of twoâ€dimensional TiSe2 on the thermoelectric, electronic and optical response of Yb14MnSb11/AlSb9Yb11 heterostructures â€ A theoretical study. Journal of Molecular Graphics and Modelling, 2019, 86, 179-191.	1.3	3

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37	Probing the nature of the Co(III) ion in corrins: The reactions of aquacyano-5-seco-cobyrinic acid heptamethyl ester with anionic ligands. Inorganica Chimica Acta, 2019, 484, 402-413.	1.2	2
38	N-doped ZnO/graphene oxide: a photostable photocatalyst for improved mineralization and photodegradation of organic dye under visible light. Ionics, 2019, 25, 327-339.	1.2	43
39	PEGylated MoS2 Nanosheets: A Dual Functional Photocatalyst for Photodegradation of Organic Dyes and Photoreduction of Chromium from Aqueous Solution. Bulletin of Chemical Reaction Engineering and Catalysis, 2019, 14, 142-152.	0.5	21
40	Photodegradation of Eosin Yellow Dye in Water under Simulated Solar Light Irradiation Using Laâ€“Doped ZnO Nanostructure Decorated on Graphene Oxide as an Advanced Photocatalyst. ChemistrySelect, 2018, 3, 1180-1188.	0.7	23
41	Tuning the electronic structures, work functions, optical properties and stability of bifunctional hybrid graphene oxide/Vâ€“doped NaNbO3 typeâ€“II heterostructures: A promising photocatalyst for H2 production. Carbon, 2018, 136, 187-195.	5.4	36
42	Understanding the synergistic effects, optical and electronic properties of ternary Fe/C/Sâ€doped TiO₂ anatase within the DFT + U approach. International Journal of Quantum Chemistry, 2018, 118, e25505.	1.0	12
43	Insights into the photocatalytic mechanism of mediator-free direct Z-scheme g-C3N4/Bi2MoO6(010) and g-C3N4/Bi2WO6(010) heterostructures: A hybrid density functional theory study. Applied Surface Science, 2018, 427, 487-498.	3.1	125
44	Dendrimer supported Fe/Ni bimetallic composites immobilized in polyethersulfone membranes for effective degradation of arginine containing microcystins. European Polymer Journal, 2018, 98, 456-467.	2.6	5
45	DMol 3 /COSMO-RS prediction of aqueous solubility and reactivity of selected Azo dyes: Effect of global orbital cut-off and COSMO segment variation. Journal of Molecular Liquids, 2018, 249, 346-360.	2.3	22
46	DFT Study of Skutterudite CoSb₃ and In_{0.2}Co₄Sb₁₂ Thermoelectric Heterostructures with 2Dâ€“WSe₂. ChemistrySelect, 2018, 3, 9336-9347.	0.7	3
47	Hybrid DFT study of MWCNT/Zr-doped SrTiO3 heterostructure: Hydrogen production, electronic properties and charge Carrier mediator role of Zr4+Âion. International Journal of Hydrogen Energy, 2018, 43, 22253-22264.	3.8	11
48	A DFT Study of Disperse Yellow 119 Degradation Mechanism by Hydroxyl Radical Attack. ChemistrySelect, 2018, 3, 12988-12997.	0.7	7
49	A first-principles study of half-Heusler intermetallic compound MgAgAs with 2D-TiC/2D-Mo2TiC composite material. Theoretical Chemistry Accounts, 2018, 137, 1.	0.5	1
50	Synergistic effect of opposite polar substituents on selected properties of disperse yellow 119 dye. Chemical Physics Letters, 2018, 704, 55-61.	1.2	3
51	Recent advances in titanium dioxide/graphene photocatalyst materials as potentials of energy generation. Bulletin of Materials Science, 2018, 41, 1.	0.8	12
52	Hierarchically Assembled Twoâ€dimensional Hybrid Nanointerfaces: A Platform for Bioelectronic Applications. Electroanalysis, 2018, 30, 2339-2348.	1.5	13
53	Graft Gum Ghatti Caped Cu2O Nanocomposite for Photocatalytic Degradation of Naphthol Blue Black Dye. Journal of Inorganic and Organometallic Polymers and Materials, 2018, 28, 1540-1551.	1.9	13
54	Theoretical studies of the interfacial charge transfer and the effect of vdW correction on the interaction energy of non-metal doped ZnO and graphene oxide interface. Theoretical Chemistry Accounts, 2018, 137, 1.	0.5	8

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55	The generation of charge carriers in semi conductors â€“ A theoretical study. Chemical Physics Letters, 2017, 678, 167-176.	1.2	16
56	Simulation from the first principal theory on the effect of supporting silica on graphene and the new composite material. Chemical Physics Letters, 2017, 680, 69-77.	1.2	7
57	Recent Progress in the Development of Semiconductorâ€Based Photocatalyst Materials for Applications in Photocatalytic Water Splitting and Degradation of Pollutants. Advanced Sustainable Systems, 2017, 1, 1700006.	2.7	144
58	Recent progress in gelatin hydrogel nanocomposites for water purification and beyond. Vacuum, 2017, 146, 396-408.	1.6	113
59	Charge transport, interfacial interactions and synergistic mechanisms in BiNbO₄/MWO₄ (M = Zn and Cd) heterostructures for hydrogen production: insights from a DFT+U study. Physical Chemistry Chemical Physics, 2017, 19, 28401-28413.	1.3	19
60	Enhancing photocatalytic activity for hydrogen production and pollutant degradation by modifying tetragonal ZrO2 with monolayers slab surface of BiVO4, Ag3PO4, SrTiO3 and WO3: A first-principles study. Computational Materials Science, 2017, 138, 462-473.	1.4	16
61	Enhancing Charge Separation and Photocatalytic Activity of Cubic SrTiO₃ withÂPerovskiteâ€Type Materials MTaO₃ (M=Na, K) for Environmental Remediation: A Firstâ€Principles Study. ChemistrySelect, 2017, 2, 6304-6316.	0.7	29
62	Progress in lignin hydrogels and nanocomposites for water purification: Future perspectives. Vacuum, 2017, 146, 342-355.	1.6	138
63	Understanding the mechanism of enhanced charge separation and visible light photocatalytic activity of modified wurtzite ZnO with nanoclusters of ZnS and graphene oxide: from a hybrid density functional study. New Journal of Chemistry, 2017, 41, 8140-8155.	1.4	69
64	Optical fibre based non-enzymatic glucose sensing over Cu2+-doped polyaniline hybrid matrix. Sensors and Actuators B: Chemical, 2017, 242, 522-528.	4.0	25
65	Synthesis and characterisation of neodymium doped-zinc oxideâ€“graphene oxide nanocomposite as a highly efficient photocatalyst for enhanced degradation of indigo carmine in water under simulated solar light. Research on Chemical Intermediates, 2017, 43, 481-501.	1.3	28
66	Role of MoS₂and WS₂monolayers on photocatalytic hydrogen production and the pollutant degradation of monoclinic BiVO₄: a first-principles study. New Journal of Chemistry, 2017, 41, 11701-11713.	1.4	48
67	Chitosanâ€“sodium alginate encapsulated Co-doped ZrO2â€“MWCNTs nanocomposites for photocatalytic decolorization of organic dyes. Research on Chemical Intermediates, 2016, 42, 7231-7245.	1.3	13
68	Palladium-dopedâ€“ZrO2â€“multiwalled carbon nanotubes nanocomposite: an advanced photocatalyst for water treatment. Applied Physics A: Materials Science and Processing, 2016, 122, 1.	1.1	19
69	Cobalt doped ZrO2 decorated multiwalled carbon nanotube: A promising nanocatalyst for photodegradation of indigo carmine and eosin Y dyes. Progress in Natural Science: Materials International, 2016, 26, 354-361.	1.8	57
70	Biodegradable polymeric nanostructures in therapeutic applications: opportunities and challenges. RSC Advances, 2016, 6, 94325-94351.	1.7	51
71	Influence of ZnO concentration on the optical and photocatalytic properties of Ni-doped ZnS/ZnO nanocomposite. Bulletin of Materials Science, 2016, 39, 1745-1752.	0.8	6
72	Photocatalytic degradation of indigo carmine using Nd-doped TiO2-decorated graphene oxide nanocomposites. Journal of Sol-Gel Science and Technology, 2016, 80, 38-49.	1.1	42

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73	Probing the nature of the Co(III) ion in cobalamins: The ligand substitution reactions of aquacyanocobester, aquacyano(10-nitro)cobester and aquacyano(10-amino)cobester. Inorganica Chimica Acta, 2016, 450, 269-278.	1.2	7
74	A resistive type humidity sensor based on crystalline tin oxide nanoparticles encapsulated in polyaniline matrix. Mikrochimica Acta, 2016, 183, 573-580.	2.5	80
75	Geochemical modelling and speciation studies of metal pollutants present in selected water systems in South Africa. Physics and Chemistry of the Earth, 2016, 92, 44-51.	1.2	10
76	Comparative photocatalytic degradation of monoazo and diazo dyes under simulated visible light using Fe3+/C/S doped-TiO2 nanoparticles. Acta Chimica Slovenica, 2016, 63, 380-391.	0.2	37
77	Neodymium Doped ZrO2-graphene Oxide Nanocomposites: A Promising Photocatalyst For Photodegradation Of Eosin Y Dye. Advanced Materials Letters, 2016, 7, 946-950.	0.3	15
78	Probing the nature of the Co(III) ion in cobalamins: The reactions of aquacobalamin (vitamin B12a), aqua-10-chlorocobalamin and aqua-10-bromocobalamin with anionic and neutral ligands. Inorganica Chimica Acta, 2015, 436, 29-38.	1.2	6
79	The Synthesis of a Corrole Analogue of Aquacobalamin (Vitamin B_{12a}) and Its Ligand Substitution Reactions. Inorganic Chemistry, 2014, 53, 4418-4429.	1.9	9
80	Phosphorylated multiwalled carbon nanotube-cyclodextrin polymer: Synthesis, characterisation and potential application in water purification. Carbohydrate Polymers, 2013, 98, 470-476.	5.1	38
81	DFT Studies of Trans and Cis Influences in the Homolysis of the Coâ€“C Bond in Models of the Alkylcobalamins. Journal of Physical Chemistry A, 2013, 117, 3057-3068.	1.1	19
82	cis Influence in Models of Cobalt Corrins by DFT and TD-DFT Studies. Journal of Physical Chemistry B, 2012, 116, 8836-8845.	1.2	18
83	The cis influence of the corrin in vitamin B12 models. Chemical Physics Letters, 2012, 550, 150-155.	1.2	8
84	Analysis of the conformational profile of trishomocubane amino acid dipeptide. Biopolymers, 2006, 81, 339-349.	1.2	17