

Penny P Govender

List of Publications by Year in descending order

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84
papers

2,235
citations

279487

23
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243296

44
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85
all docs

85
docs citations

85
times ranked

3168
citing authors

#	ARTICLE	IF	CITATIONS
1	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. <i>Journal of Molecular Liquids</i> , 2020, 298, 112040.	2.3	319
2	Recent Progress in the Development of Semiconductor-Based Photocatalyst Materials for Applications in Photocatalytic Water Splitting and Degradation of Pollutants. <i>Advanced Sustainable Systems</i> , 2017, 1, 1700006.	2.7	144
3	Progress in lignin hydrogels and nanocomposites for water purification: Future perspectives. <i>Vacuum</i> , 2017, 146, 342-355.	1.6	138
4	Insights into the photocatalytic mechanism of mediator-free direct Z-scheme g-C ₃ N ₄ /Bi ₂ MoO ₆ (010) and g-C ₃ N ₄ /Bi ₂ WO ₆ (010) heterostructures: A hybrid density functional theory study. <i>Applied Surface Science</i> , 2018, 427, 487-498.	3.1	125
5	Recent progress in gelatin hydrogel nanocomposites for water purification and beyond. <i>Vacuum</i> , 2017, 146, 396-408.	1.6	113
6	A resistive type humidity sensor based on crystalline tin oxide nanoparticles encapsulated in polyaniline matrix. <i>Mikrochimica Acta</i> , 2016, 183, 573-580.	2.5	80
7	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. <i>New Journal of Chemistry</i> , 2017, 41, 8140-8155.	1.4	69
8	MoS ₂ Nanosheet/ZnS Composites for the Visible-Light-Assisted Photocatalytic Degradation of Oxytetracycline. <i>ACS Applied Nano Materials</i> , 2021, 4, 4721-4734.	2.4	61
9	Tuning the electronic and structural properties of Gd-TiO ₂ -GO nanocomposites for enhancing photodegradation of IC dye: The role of Gd ³⁺ ion. <i>Applied Catalysis B: Environmental</i> , 2019, 243, 106-120.	10.8	60
10	Cobalt doped ZrO ₂ decorated multiwalled carbon nanotube: A promising nanocatalyst for photodegradation of indigo carmine and eosin Y dyes. <i>Progress in Natural Science: Materials International</i> , 2016, 26, 354-361.	1.8	57
11	Biodegradable polymeric nanostructures in therapeutic applications: opportunities and challenges. <i>RSC Advances</i> , 2016, 6, 94325-94351.	1.7	51
12	Role of MoS ₂ and WS ₂ monolayers on photocatalytic hydrogen production and the pollutant degradation of monoclinic BiVO ₄ : a first-principles study. <i>New Journal of Chemistry</i> , 2017, 41, 11701-11713.	1.4	48
13	N-doped ZnO/graphene oxide: a photostable photocatalyst for improved mineralization and photodegradation of organic dye under visible light. <i>Ionics</i> , 2019, 25, 327-339.	1.2	43
14	Photocatalytic degradation of indigo carmine using Nd-doped TiO ₂ -decorated graphene oxide nanocomposites. <i>Journal of Sol-Gel Science and Technology</i> , 2016, 80, 38-49.	1.1	42
15	Phosphorylated multiwalled carbon nanotube-cyclodextrin polymer: Synthesis, characterisation and potential application in water purification. <i>Carbohydrate Polymers</i> , 2013, 98, 470-476.	5.1	38
16	Comparative photocatalytic degradation of monoazo and diazo dyes under simulated visible light using Fe ³⁺ /C/S doped-TiO ₂ nanoparticles. <i>Acta Chimica Slovenica</i> , 2016, 63, 380-391.	0.2	37
17	Tuning the electronic structures, work functions, optical properties and stability of bifunctional hybrid graphene oxide/V ⁿ⁺ -doped NaNbO ₃ type-II heterostructures: A promising photocatalyst for H ₂ production. <i>Carbon</i> , 2018, 136, 187-195.	5.4	36
18	Enhancing Charge Separation and Photocatalytic Activity of Cubic SrTiO ₃ with Perovskite-Type Materials MTaO ₃ (M=Na, K) for Environmental Remediation: A First-Principles Study. <i>ChemistrySelect</i> , 2017, 2, 6304-6316.	0.7	29

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19	Highly Selective and Sensitive Detection of Formaldehyde by I_2 -Borophene/SnO ₂ Heterostructures: The Role of an External Electric Field and In-Plane Biaxial Strain. <i>Journal of Physical Chemistry A</i> , 2020, 124, 2288-2300.	1.1	29
20	Developing a simple box-behken experimental design on the removal of doxorubicin anticancer drug using Fe ₃ O ₄ /graphene nanoribbons adsorbent. <i>Environmental Research</i> , 2021, 200, 111522.	3.7	29
21	Synthesis and characterisation of neodymium doped-zinc oxide-graphene oxide nanocomposite as a highly efficient photocatalyst for enhanced degradation of indigo carmine in water under simulated solar light. <i>Research on Chemical Intermediates</i> , 2017, 43, 481-501.	1.3	28
22	Optical fibre based non-enzymatic glucose sensing over Cu ²⁺ -doped polyaniline hybrid matrix. <i>Sensors and Actuators B: Chemical</i> , 2017, 242, 522-528.	4.0	25
23	Adsorption behaviour of Si anchored on g-C ₃ N ₄ /graphene van der Waals heterostructure for selective sensing of toxic gases: Insights from a first-principles study. <i>Applied Surface Science</i> , 2020, 525, 146590.	3.1	24
24	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. <i>Journal of Molecular Liquids</i> , 2020, 311, 113314.	2.3	24
25	Photodegradation of Eosin Yellow Dye in Water under Simulated Solar Light Irradiation Using La-Doped ZnO Nanostructure Decorated on Graphene Oxide as an Advanced Photocatalyst. <i>ChemistrySelect</i> , 2018, 3, 1180-1188.	0.7	23
26	DMol 3 /COSMO-RS prediction of aqueous solubility and reactivity of selected Azo dyes: Effect of global orbital cut-off and COSMO segment variation. <i>Journal of Molecular Liquids</i> , 2018, 249, 346-360.	2.3	22
27	PEGylated MoS ₂ Nanosheets: A Dual Functional Photocatalyst for Photodegradation of Organic Dyes and Photoreduction of Chromium from Aqueous Solution. <i>Bulletin of Chemical Reaction Engineering and Catalysis</i> , 2019, 14, 142-152.	0.5	21
28	DFT Studies of Trans and Cis Influences in the Homolysis of the Co-C Bond in Models of the Alkylcobalamins. <i>Journal of Physical Chemistry A</i> , 2013, 117, 3057-3068.	1.1	19
29	Palladium-doped-ZrO ₂ -multiwalled carbon nanotubes nanocomposite: an advanced photocatalyst for water treatment. <i>Applied Physics A: Materials Science and Processing</i> , 2016, 122, 1.	1.1	19
30	Charge transport, interfacial interactions and synergistic mechanisms in BiNbO ₄ /MWO ₄ (M = Zn and Cd) heterostructures for hydrogen production: insights from a DFT+U study. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 28401-28413.	1.3	19
31	cis Influence in Models of Cobalt Corrins by DFT and TD-DFT Studies. <i>Journal of Physical Chemistry B</i> , 2012, 116, 8836-8845.	1.2	18
32	Experimental and Computational Design of Highly Active Ce-ZrO ₂ -GO Photocatalyst for Eosin Yellow Dye Degradation: The Role of Interface and Ce ³⁺ Ion. <i>Catalysis Letters</i> , 2019, 149, 1633-1650.	1.4	18
33	Analysis of the conformational profile of trishomocubane amino acid dipeptide. <i>Biopolymers</i> , 2006, 81, 339-349.	1.2	17
34	The generation of charge carriers in semi conductors - A theoretical study. <i>Chemical Physics Letters</i> , 2017, 678, 167-176.	1.2	16
35	Enhancing photocatalytic activity for hydrogen production and pollutant degradation by modifying tetragonal ZrO ₂ with monolayers slab surface of BiVO ₄ , Ag ₃ PO ₄ , SrTiO ₃ and WO ₃ : A first-principles study. <i>Computational Materials Science</i> , 2017, 138, 462-473.	1.4	16
36	Tuning the electronic, optical and structural properties of GaS/C ₂ N van der Waals heterostructure for photovoltaic application: first-principle calculations. <i>SN Applied Sciences</i> , 2020, 2, 1.	1.5	16

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37	Electrochemical Detection of Tetracycline on Highly Sensitive Benzene Sourced CVD Graphene-Gold Nanoparticles Nanointerfaces. <i>Electroanalysis</i> , 2021, 33, 412-420.	1.5	16
38	Insights into the complementary behaviour of Gd doping in GO/Gd/ZnO composites as an efficient candidate towards photocatalytic degradation of indigo carmine dye. <i>Journal of Materials Science</i> , 2021, 56, 8511-8527.	1.7	16
39	Neodymium Doped ZrO ₂ -graphene Oxide Nanocomposites: A Promising Photocatalyst For Photodegradation Of Eosin Y Dye. <i>Advanced Materials Letters</i> , 2016, 7, 946-950.	0.3	15
40	Switchable Graphene-Based Bioelectronics Interfaces. <i>Chemosensors</i> , 2020, 8, 45.	1.8	14
41	Remarkable Enhancement of Eu-TiO ₂ -GO Composite for Photodegradation of Indigo Carmine: A Design Method Based on Computational and Experimental Perspectives. <i>Catalysis Letters</i> , 2021, 151, 1111-1126.	1.4	14
42	Chitosan-sodium alginate encapsulated Co-doped ZrO ₂ -MWCNTs nanocomposites for photocatalytic decolorization of organic dyes. <i>Research on Chemical Intermediates</i> , 2016, 42, 7231-7245.	1.3	13
43	Hierarchically Assembled Two-dimensional Hybrid Nanointerfaces: A Platform for Bioelectronic Applications. <i>Electroanalysis</i> , 2018, 30, 2339-2348.	1.5	13
44	Graft Gum Ghatti Caped Cu ₂ O Nanocomposite for Photocatalytic Degradation of Naphthol Blue Black Dye. <i>Journal of Inorganic and Organometallic Polymers and Materials</i> , 2018, 28, 1540-1551.	1.9	13
45	Evaluating Iso-Mukaadial Acetate and Ursolic Acid Acetate as Plasmodium falciparum Hypoxanthine-Guanine-Xanthine Phosphoribosyltransferase Inhibitors. <i>Biomolecules</i> , 2019, 9, 861.	1.8	13
46	Understanding the synergistic effects, optical and electronic properties of ternary Fe/C-doped TiO ₂ anatase within the DFT approach. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25505.	1.0	12
47	Recent advances in titanium dioxide/graphene photocatalyst materials as potentials of energy generation. <i>Bulletin of Materials Science</i> , 2018, 41, 1.	0.8	12
48	Ligand-based pharmacophore modelling and virtual screening for the identification of amyloid-beta diagnostic molecules. <i>Journal of Molecular Graphics and Modelling</i> , 2020, 101, 107711.	1.3	12
49	Electrochemical detection of amoxicillin on 2D graphene-gold nanoparticle-Lacasse bio-interfaces: Combined experimental and theoretical study. <i>Chemical Physics Letters</i> , 2021, 764, 138278.	1.2	12
50	Hybrid DFT study of MWCNT/Zr-doped SrTiO ₃ heterostructure: Hydrogen production, electronic properties and charge Carrier mediator role of Zr ⁴⁺ ion. <i>International Journal of Hydrogen Energy</i> , 2018, 43, 22253-22264.	3.8	11
51	Geochemical modelling and speciation studies of metal pollutants present in selected water systems in South Africa. <i>Physics and Chemistry of the Earth</i> , 2016, 92, 44-51.	1.2	10
52	One-step synthesized 2D heteroatom doped graphene for high throughput electrochemical biosensing: A combined experimental and computational studies. <i>Diamond and Related Materials</i> , 2019, 100, 107592.	1.8	10
53	Computational investigation of the binding characteristics of I ² -amyloid fibrils. <i>Biophysical Chemistry</i> , 2020, 256, 106281.	1.5	10
54	The Synthesis of a Corrole Analogue of Aquacobalamin (Vitamin B _{12a}) and Its Ligand Substitution Reactions. <i>Inorganic Chemistry</i> , 2014, 53, 4418-4429.	1.9	9

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55	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. <i>Theoretical Chemistry Accounts</i> , 2019, 138, 1.	0.5	9
56	Tuning the electronic properties and interfacial interactions of WS ₂ /ZrO ₂ (001) heterostructures by an external electric field, interlayer coupling and monolayer to few-layer of WS ₂ sheets. <i>Materials Chemistry and Physics</i> , 2019, 224, 107-116.	2.0	9
57	Hierarchically assembled two-dimensional gold boron nitride-tungsten disulphide nanohybrid interface system for electrobiocatalytic applications. <i>Materials Chemistry and Physics</i> , 2019, 226, 129-140.	2.0	9
58	The cis influence of the corrin in vitamin B12 models. <i>Chemical Physics Letters</i> , 2012, 550, 150-155.	1.2	8
59	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. <i>Theoretical Chemistry Accounts</i> , 2018, 137, 1.	0.5	8
60	Two-dimensional CoOOH as a Highly Sensitive and Selective H ₂ S, HCN and HF Gas Sensor: A Computational Investigation. <i>Electroanalysis</i> , 2020, 32, 2764-2774.	1.5	8
61	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. <i>Inorganica Chimica Acta</i> , 2016, 450, 269-278.	1.2	7
62	Simulation from the first principal theory on the effect of supporting silica on graphene and the new composite material. <i>Chemical Physics Letters</i> , 2017, 680, 69-77.	1.2	7
63	A DFT Study of Disperse Yellow 119 Degradation Mechanism by Hydroxyl Radical Attack. <i>ChemistrySelect</i> , 2018, 3, 12988-12997.	0.7	7
64	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. <i>Inorganica Chimica Acta</i> , 2015, 436, 29-38.	1.2	6
65	Influence of ZnO concentration on the optical and photocatalytic properties of Ni-doped ZnS/ZnO nanocomposite. <i>Bulletin of Materials Science</i> , 2016, 39, 1745-1752.	0.8	6
66	Dendrimer supported Fe/Ni bimetallic composites immobilized in polyethersulfone membranes for effective degradation of arginine containing microcystins. <i>European Polymer Journal</i> , 2018, 98, 456-467.	2.6	5
67	High-Throughput 2D Heteroatom Graphene Bioelectronic Nanosculpture: A Combined Experimental and Theoretical Study. <i>ACS Applied Materials & Interfaces</i> , 2019, 11, 11238-11250.	4.0	5
68	Thermoelectric, Electronic, and Optical Response of Nanostructured Al-doped ZnO @ 2D-TiC Composite. <i>ChemistrySelect</i> , 2020, 5, 13144-13154.	0.7	5
69	Exploring the Optical, Structural and Electronic Properties of a Two-Dimensional GaSe/C ₂ N van der Waals Heterostructure As a Photovoltaic Cell: A Computational Investigation. <i>Journal of Electronic Materials</i> , 2021, 50, 620-628.	1.0	5
70	Imidazolium-Quaternized Poly(2,6-Dimethyl-1,4-Phenylene Oxide)/Zeolitic Imidazole Framework-8 Composite Membrane as Polymer Electrolyte for Fuel-Cell Application. <i>Polymers</i> , 2022, 14, 595.	2.0	5
71	Tuning the aqueous solubility, chemical reactivity and absorption wavelength of azo dye through systematic adjustment of molecular charge density: a DFT study. <i>Molecular Physics</i> , 2020, 118, .	0.8	4
72	Electro-catalytic amplified sensor for determination of N-acetylcysteine in the presence of theophylline confirmed by experimental coupled theoretical investigation. <i>Scientific Reports</i> , 2021, 11, 1006.	1.6	4

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73	DFT Study of Skutterudite CoSb_3 and $\text{In}_{0.2}\text{Co}_4\text{Sb}_{12}$ Thermoelectric Heterostructures with 2D WSe_2 . ChemistrySelect, 2018, 3, 9336-9347.	0.7	3
74	Synergistic effect of opposite polar substituents on selected properties of disperse yellow 119 dye. Chemical Physics Letters, 2018, 704, 55-61.	1.2	3
75	The effects of two-dimensional TiSe_2 on the thermoelectric, electronic and optical response of $\text{Yb}_{14}\text{MnSb}_{11}/\text{AlSb}_9\text{Yb}_{11}$ heterostructures – A theoretical study. Journal of Molecular Graphics and Modelling, 2019, 86, 179-191.	1.3	3
76	Composite 2D Nanointerfaces for Electrochemical Biosensing: An Experimental and Theoretical Study. ACS Applied Bio Materials, 2020, 3, 8676-8687.	2.3	3
77	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
78	In vitro and in silico studies of the antifungal properties of the bulb and leaves extracts of <i>Drimia delagoensis</i> Baker (Jessop). Advances in Traditional Medicine, 2020, 20, 373-379.	1.0	2
79	A first-principles study of half-Heusler intermetallic compound MgAgAs with 2D- $\text{TiC}/2\text{D-Mo}_2\text{TiC}$ composite material. Theoretical Chemistry Accounts, 2018, 137, 1.	0.5	1
80	A theoretical study of 2D AlN on 3D $\text{C}_4\text{H}_6\text{N}_6\text{Ni}_2$ clathrate thermoelectric material composites. SN Applied Sciences, 2019, 1, 1.	1.5	1
81	Computational screening of vdWs heterostructures of BSe with MoSe_2 and WSe_2 as sustainable hydrogen production materials. Current Applied Physics, 2020, , .	1.1	1
82	Prospective of functionalized nanomaterials in environmental science: A nanotechnological approach. , 2021, , 13-60.		1
83	SF_6 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
84	Atomistic insight into the significantly enhanced photovoltaic cells of monolayer GaTe_2 via two-dimensional van der Waals heterostructures engineering. ChemistrySelect, 2022, 7, 629-644.	0.7	0