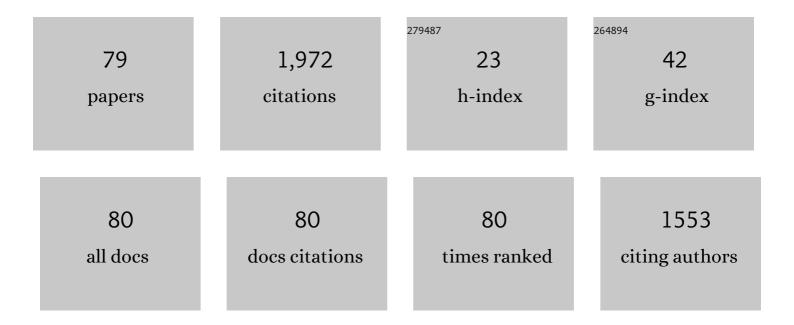
List of Publications by Year in descending order

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DERNADAVAN IANA

#	Article	IF	CITATIONS
1	Effect of chemical doping of boron and nitrogen on the electronic, optical, and electrochemical properties of carbon nanotubes. Progress in Materials Science, 2013, 58, 565-635.	16.0	276
2	Ab-initio calculation of electronic and optical properties of nitrogen and boron doped graphene nanosheet. Carbon, 2014, 73, 275-282.	5.4	165
3	A theoretical review on electronic, magnetic and optical properties of silicene. Reports on Progress in Physics, 2016, 79, 126501.	8.1	155
4	Engineering of ZnO/rGO nanocomposite photocatalyst towards rapid degradation of toxic dyes. Materials Chemistry and Physics, 2019, 223, 456-465.	2.0	123
5	Optical properties of P and Al doped silicene: a first principles study. RSC Advances, 2015, 5, 41-50.	1.7	52
6	Semi-metallic to semiconducting transition in graphene nanosheet with site specific co-doping of boron and nitrogen. Physica E: Low-Dimensional Systems and Nanostructures, 2014, 56, 64-68.	1.3	50
7	A review on role of tetra-rings in graphene systems and their possible applications. Reports on Progress in Physics, 2020, 83, 056501.	8.1	47
8	Size dependent magnetic and optical properties in diamond shaped graphene quantum dots: A DFT study. Journal of Physics and Chemistry of Solids, 2016, 99, 34-42.	1.9	46
9	Defect induced magnetism in planar silicene: a first principles study. RSC Advances, 2014, 4, 32221.	1.7	44
10	A first principles study of the optical properties of BxCy single wall nanotubes. Carbon, 2007, 45, 1482-1491.	5.4	41
11	First principles calculations of the optical properties of CxNysingle walled nanotubes. Nanotechnology, 2009, 20, 175701.	1.3	41
12	Twin T-graphene: a new semiconducting 2D carbon allotrope. Physical Chemistry Chemical Physics, 2020, 22, 10286-10294.	1.3	39
13	Acetylenic linkage dependent electronic and optical behaviour of morphologically distinct â€~-ynes'. Physical Chemistry Chemical Physics, 2019, 21, 13795-13808.	1.3	37
14	The topology and robustness of two Dirac cones in S-graphene: A tight binding approach. Scientific Reports, 2020, 10, 2502.	1.6	34
15	Efficient Flexible White-Light Photodetectors Based on BiFeO ₃ Nanoparticles. ACS Applied Nano Materials, 2018, 1, 625-631.	2.4	33
16	Electric field induced band tuning, optical and thermoelectric responses in tetragonal germanene: a theoretical approach. Physical Chemistry Chemical Physics, 2020, 22, 19957-19968.	1.3	31
17	A real-space study of random extended defects in solids: Application to disordered Stone–Wales defects in graphene. Physica E: Low-Dimensional Systems and Nanostructures, 2014, 61, 191-197.	1.3	29
18	Optical properties and magnetic flux-induced electronic band tuning of a T-graphene sheet and nanoribbon. Physical Chemistry Chemical Physics, 2017, 19, 21584-21594.	1.3	28

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19	Tetragonal graphene nanodot as carbon monoxide gas sensor and current rectification device. Journal of Physics and Chemistry of Solids, 2018, 123, 172-182.	1.9	27
20	Emerging properties of carbon based 2D material beyond graphene. Journal of Physics Condensed Matter, 2022, 34, 053001.	0.7	27
21	Electronic and optical properties of non-hexagonal Dirac material S-graphene sheet and nanoribbons. Physica E: Low-Dimensional Systems and Nanostructures, 2020, 120, 114087.	1.3	26
22	8-16-4 graphyne: Square-lattice two-dimensional nodal line semimetal with a nontrivial topological Zak index. Physical Review B, 2021, 103, .	1.1	26
23	General strategies to improve thermoelectric performance with an emphasis on tin and germanium chalcogenides as thermoelectric materials. Journal of Materials Chemistry A, 2022, 10, 6872-6926.	5.2	26
24	Nitrogenated CQD decorated ZnO nanorods towards rapid photodegradation of rhodamine B: A combined experimental and theoretical approach. Applied Surface Science, 2021, 563, 150315.	3.1	25
25	Ab-initio calculation of optical properties of AA-stacked bilayer graphene with tunable layer separation. Current Applied Physics, 2015, 15, 691-697.	1.1	24
26	Impressive Thermoelectric Figure of Merit in Two-Dimensional Tetragonal Pnictogens: a Combined First-Principles and Machine-Learning Approach. ACS Applied Materials & Interfaces, 2021, 13, 59092-59103.	4.0	24
27	Beyond T-graphene: Two-dimensional tetragonal allotropes and their potential applications. Applied Physics Reviews, 2022, 9, .	5.5	23
28	Search for magnetism in transition metal atoms doped tetragonal graphene: A DFT approach. Journal of Magnetism and Magnetic Materials, 2017, 441, 523-530.	1.0	21
29	Strain induced electronic and magnetic properties of 2D magnet Crl ₃ : a DFT approach. Journal of Physics Condensed Matter, 2019, 31, 335802.	0.7	21
30	Electronic and optical properties of the supercell of 8-Pmmn borophene modified on doping by H, Li, Be, and C: a DFT approach. Applied Physics A: Materials Science and Processing, 2019, 125, 1.	1.1	21
31	Half metallic ferromagnetic and optical properties of ruthenium-doped zincblende ZnS: A first principles study. Journal of Physics and Chemistry of Solids, 2020, 136, 109175.	1.9	21
32	Tuning electronic, magnetic and optical properties of germanene nanosheet with site dependent adatoms arsenic and gallium: A first principles study. Current Applied Physics, 2017, 17, 573-583.	1.1	20
33	First-principles calculation of the electronic and optical properties of a new two-dimensional carbon allotrope: tetra-penta-octagonal graphene. Physical Chemistry Chemical Physics, 2019, 21, 24758-24767.	1.3	20
34	Optical properties of transition metal atom adsorbed graphene: A density functional theoretical calculation. Physica E: Low-Dimensional Systems and Nanostructures, 2015, 69, 306-315.	1.3	19
35	Exploring the role of electronic structure on photo-catalytic behavior of carbon-nitride polymorphs. Carbon, 2020, 168, 125-134.	5.4	19
36	TPDH-graphene: A new two dimensional metallic carbon with NDR behaviour of its one dimensional derivatives. Physica E: Low-Dimensional Systems and Nanostructures, 2021, 127, 114569.	1.3	19

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37	Electronic and thermal transport in novel carbon-based bilayer with tetragonal rings: a combined study using first-principles and machine learning approach. Physical Chemistry Chemical Physics, 2021, 23, 14608-14616.	1.3	19
38	First principles Raman study of boron and nitrogen doped planar T-graphene clusters. Materials Research Express, 2015, 2, 095603.	0.8	18
39	Effect of beryllium doping and vacancy in band structure, magnetic and optical properties of free standing germanene. Current Applied Physics, 2017, 17, 1589-1600.	1.1	18
40	Shape dependent magnetic and optical properties in silicene nanodisks: A first principles study. Journal of Physics and Chemistry of Solids, 2015, 83, 32-39.	1.9	17
41	Magnetic and optical properties of carbon and silicon decorated free standing buckled germanene: A DFT approach. Journal of Physics and Chemistry of Solids, 2018, 115, 332-341.	1.9	15
42	First-principles study of the optical and thermoelectric properties of tetragonal-silicene. Physical Chemistry Chemical Physics, 2021, 23, 11863-11875.	1.3	14
43	First principles investigation of structural, electronic and optical properties of synthesized radiaannulene oligomers for 6,6,12-graphyne. Journal of Physics and Chemistry of Solids, 2021, 153, 109990.	1.9	13
44	Mechanical characteristics and electric field-influenced thermoelectric and optical responses of tetragonal germanene. Journal Physics D: Applied Physics, 2021, 54, 405303.	1.3	12
45	Visible LEDâ€Assisted Effective Charge Separation in Rutheniumâ€Doped ZnS System for Efficient Photodegradation of Organic Dye. ChemistrySelect, 2019, 4, 9102-9111.	0.7	11
46	Effect and Characterization of Stone–Wales Defects on Graphene Quantum Dot: A First-Principles Study. Condensed Matter, 2018, 3, 50.	0.8	10
47	Tetragonal Silicene and Germanene Quantum Dots: Candidates for Enhanced Nonlinear Optical and Photocatalytic Activity. Journal of Physical Chemistry C, 2021, 125, 21718-21728.	1.5	10
48	Intriguing features of Dirac cones in phagraphene with site specific doping. Applied Surface Science, 2021, 577, 151782.	3.1	10
49	An ab-initio approach to the optical properties of CxNy single wall nanotubes. Diamond and Related Materials, 2009, 18, 1002-1005.	1.8	9
50	Electronic and magnetic properties of modified silicene/graphene hybrid: Ab initio study. Materials Chemistry and Physics, 2016, 183, 580-587.	2.0	9
51	Conductance of disordered graphene sheets: A real space approach. Physica E: Low-Dimensional Systems and Nanostructures, 2015, 74, 347-354.	1.3	8
52	Electronic structural critique of interesting thermal and optical properties of C ₁₇ Ge germagraphene. Physical Chemistry Chemical Physics, 2020, 22, 8606-8615.	1.3	8
53	A complete theory for the magnetism of an ideal gas of electrons. Physics of Plasmas, 2013, 20, .	0.7	7
54	Configuration and self-averaging in disordered systems. Indian Journal of Physics, 2016, 90, 649-657.	0.9	7

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55	Excess energy of an ultracold Fermi gas in a trapped geometry. European Physical Journal D, 2012, 66, 1.	0.6	6
56	Kardar–Parisi–Zhang universality class of a discrete erosion model. International Journal of Modern Physics C, 2015, 26, 1550049.	0.8	6
57	A first principles approach to magnetic and optical properties in single-layer graphene sandwiched between boron nitride monolayers. Materials Research Express, 2015, 2, 075601.	0.8	6
58	Emergence of magnetic anisotropy by surface adsorption of transition metal dimers on γ-graphyne framework. Journal of Physics Condensed Matter, 2021, 33, 205501.	0.7	6
59	Combined theoretical and experimental study of the electronic and optical property of Sb2WO6. Journal of Alloys and Compounds, 2021, 881, 160586.	2.8	6
60	Electric field-induced electronic-thermoelectric-optical properties of typical isoelectronic HNC6 monolayers: A theoretical study. Applied Surface Science, 2022, 581, 152094.	3.1	5
61	Worm-graphene: A two-dimensional orthorhombic carbon semimetal with massless Dirac fermion. Applied Surface Science, 2022, 585, 152457.	3.1	5
62	Optical and magnetic properties of free-standing silicene, germanene and T-graphene system. ChemistrySelect, 2017, 2, .	0.7	4
63	Experimental evidence of multiaffinity of pinned interfaces. European Physical Journal B, 2013, 86, 1.	0.6	3
64	Modifications of optical properties in doped germanene nanosheet. International Journal of Nano and Biomaterials, 2017, 7, 29.	0.1	3
65	Effect of Annealing Temperature on the Structural and the Electrical Transport Properties of La ₂ NiMnO ₆ Nanoparticles. Physica Status Solidi (B): Basic Research, 2018, 255, 1700436.	0.7	3
66	Simple correction to bandgap problems in IV and III–V semiconductors: an improved, local first-principles density functional theory. Journal of Physics Condensed Matter, 2019, 31, 495502.	0.7	3
67	Electronic and optical properties of PTCDI adsorbed graphene heterostructure: A first principles study. Journal of Physics and Chemistry of Solids, 2021, 155, 110109.	1.9	3
68	A Comparative Study of Optical Anisotropies of BC3 and B3C Systems by Density Functional Theory. ISRN Nanotechnology, 2011, 2011, 1-9.	1.3	3
69	Effect of Co and Mg doping at Cu site on structural, magnetic and dielectric properties of α–Cu ₂ V ₂ O ₇ . Journal of Physics Condensed Matter, 2022, 34, 075702.	0.7	3
70	Optical and Thermoelectric Behavior of Phagraphene with Siteâ€ 5 pecific Bâ€N Coâ€Doping. Advanced Theory and Simulations, 2022, 5, .	1.3	3
71	One-step hydrothermal synthesis of Sb2WO6 nanoparticle towards excellent LED light driven photocatalytic dye degradation. Applied Physics A: Materials Science and Processing, 2022, 128, .	1.1	3
72	A COMPARATIVE STUDY OF OPTICAL PROPERTIES OF C3N AND CN3 SYSTEMS THROUGH DENSITY FUNCTIONAL THEORY (DFT). International Journal of Nanoscience, 2011, 10, 361-365.	0.4	2

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73	Multi-facets of kinetic roughening of interfaces. Physical Sciences Reviews, 2019, 4, .	0.8	2
74	A DFT perspective analysis of optical properties of defected germanene mono-layer. Physical Sciences Reviews, 2018, 3, .	0.8	1
75	Optical properties of monolayer BeC under an external electric field: A DFT approach. Physical Sciences Reviews, 2018, 3, .	0.8	1
76	Defects dynamics in annealed Si3N4by positron annihilation spectroscopy. Physica Status Solidi C: Current Topics in Solid State Physics, 2009, 6, 2533-2536.	0.8	0
77	Observation of nonuniversal scaling exponent in a novel erosion model. International Journal of Modern Physics C, 2015, 26, 1550115.	0.8	0
78	2. Optical and magnetic properties of free-standing silicene, germanene and T-graphene system. , 2017, , 23-70.		0
79	1. Optical properties of monolayer BeC under an external electric field: A DFT approach. , 2018, , 1-18.		0