Utpal Sarkar

List of Publications by Year
in descending order

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105	4,961	136950	95266
papers	citations	32 h-index	68 g-index

109	109	109	3377
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	High capacitance twinâ€graphene anode material for magnesium ion battery. Energy Storage, 2023, 5, .	4.3	13
2	Electronic and transport property of two-dimensional boron phosphide sheet. Journal of Molecular Graphics and Modelling, 2022, 112, 108117.	2.4	12
3	Selective N,N-Dimethylformamide Vapor Sensing Using MoSe₂/Multiwalled Carbon Nanotube Composites at Room Temperature. ACS Applied Nano Materials, 2022, 5, 3913-3924.	5.0	20
4	MoSe2/multiwalled carbon nanotube composite for ammonia sensing in natural humid environment. Journal of Hazardous Materials, 2022, 435, 128821.	12.4	29
5	Solvent Effects on the Photophysical Properties of a Donorâ€“acceptor Based Schiff Base. Journal of Fluorescence, 2022, 32, 1321-1336.	2.5	4
6	Highly Selective Ethyl Mercaptan Sensing Using a MoSe₂/SnO₂ Composite at Room Temperature. ACS Applied Materials & Interfaces, 2022, 14, 23916-23927.	8.0	20
7	Thermoelectric properties of pentagraphene. Physica B: Condensed Matter, 2022, 641, 414091.	2.7	11
8	Boron-nitride and boron-phosphide doped twin-graphene: Applications in electronics and optoelectronics. Applied Surface Science, 2021, 541, 148657.	6.1	53
9	Ultrahigh carrier mobility of penta-graphene: A first-principle study. Physica E: Low-Dimensional Systems and Nanostructures, 2021, 127, 114507.	2.7	50
10	Tuning electronic properties of bilayer Î±-graphyne by external electric field: a density functional theory study. Monatshefte FÃ¼r Chemie, 2021, 152, 61-66.	1.8	1
11	Reactivity Dynamics. Journal of Physical Chemistry A, 2021, 125, 2051-2060.	2.5	34
12	MoS₂/WO₃Nanosheets for Detection of Ammonia. ACS Applied Nano Materials, 2021, 4, 2594-2605.	5.0	80
13	Twin-graphene as a Promising Anode Material for Na-Ion Rechargeable Batteries. ACS Applied Nano Materials, 2021, 4, 4912-4918.	5.0	39
14	MoS₂/MoO₃ Nanocomposite for Selective NH₃ Detection in a Humid Environment. ACS Sustainable Chemistry and Engineering, 2021, 9, 7328-7340.	6.7	84
15	Detection of nitrobenzene using transition metal doped C24: A DFT study. Structural Chemistry, 2021, 32, 2259-2270.	2.0	26
16	Conceptual DFT based electronic structure principles in a dynamical context. Journal of the Indian Chemical Society, 2021, 98, 100098.	2.8	10
17	Thermoelectric Properties of Pristine Graphyne and the BN-Doped Graphyne Family. ACS Omega, 2021, 6, 20149-20157.	3.5	24
18	Designing nanoscale capacitors based on twin-graphene. Physical Chemistry Chemical Physics, 2021, 23, 16268-16276.	2.8	16

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19	Low-temperature nematic phase in azo functionalised reactive hockey stick mesogens possessing lateral methyl group. Dyes and Pigments, 2020, 173, 107233.	3.7	4
20	Non-covalent interactions between epinephrine and nitroaromatic compounds: A DFT study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2020, 228, 117827.	3.9	22
21	Pentagraphyne: a new carbon allotrope with superior electronic and optical property. Journal of Materials Chemistry C, 2020, 8, 16143-16150.	5.5	49
22	Penta-BeS2 monolayer: A new 2D material. AIP Conference Proceedings, 2020, , .	0.4	3
23	Confinement Effects of a Noble Gas Dimer Inside a Fullerene Cage: Can It Be Used as an Acceptor in a DSSC?. Frontiers in Chemistry, 2020, 8, 621.	3.6	13
24	Detection of NOx and COx (x = 1, 2) molecules with T4,4,4-graphyne: a density functional theory study. Molecular Simulation, 2020, 46, 1383-1389.	2.0	5
25	MoSe₂ Crystalline Nanosheets for Room-Temperature Ammonia Sensing. ACS Applied Nano Materials, 2020, 3, 9375-9384.	5.0	79
26	A Detailed DFT Study on Electronic Structures and Nonlinear Optical Properties of Doped C₃₀. ChemistrySelect, 2020, 5, 6987-6999.	1.5	22
27	Density Functional Theory Investigation of Nonlinear Optical Properties of T-Graphene Quantum Dots. Journal of Physical Chemistry A, 2020, 124, 1312-1320.	2.5	65
28	Theoretical study of electronic transport through P-porphyrin and S-porphyrin nanoribbons. Journal of Molecular Graphics and Modelling, 2020, 97, 107543.	2.4	5
29	Influence of noble gas atoms on B12N12 fullerene: A DFT study. AIP Conference Proceedings, 2019, , .	0.4	4
30	Donor-acceptor decorated graphyne: A promising candidate for nonlinear optical application. AIP Conference Proceedings, 2019, , .	0.4	8
31	Electronic and optical properties of XN-ynes (Xâ€¯=â€¯B, Al, Ga): A first-principle study with many-body effects. Applied Surface Science, 2019, 495, 143612.	6.1	31
32	Boron-phosphorous doped graphyne: A near-infrared light absorber. AIP Advances, 2019, 9, .	1.3	30
33	Interaction of a bioactive molecule with surfaces of nanoscale transition metal oxides: experimental and theoretical studies. New Journal of Chemistry, 2019, 43, 16621-16628.	2.8	4
34	Raman and IR signature of pristine and BN- doped Î³-graphyne from first-principle. Carbon, 2019, 141, 652-662.	10.3	21
35	Foreword for the Festschrift on the occasion of the 60th birthday of Professor Pratim Kumar Chattaraj. Journal of Molecular Modeling, 2019, 25, 52.	1.8	0
36	Molecular structure, chemical reactivity, nonlinear optical activity and vibrational spectroscopic density functional theory and experimental approach. Journal of Molecular Structure, 2018, 1160, 167-176.	3.6	19

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37	Electronic, nonlinear optical and thermodynamic properties of (CdS) n clusters: A first principle study. Computational Condensed Matter, 2018, 14, 40-45.	2.1	12
38	The Influence of the Substitution of Transition Metals on Pristine C₂₀: A DFT Study. International Journal of Nanoscience, 2018, 17, 1760026.	0.7	11
39	The spin filtering effect and negative differential behavior of the graphene-pentalene-graphene molecular junction: a theoretical analysis. Journal of Molecular Modeling, 2018, 24, 278.	1.8	3
40	Transition metal doped (X = V, Cr) CdS monolayer: A DFT study. AIP Conference Proceedings, 2018, , .	0.4	6
41	Optical properties of C28 fullerene cage: A DFT study. AIP Conference Proceedings, 2018, , .	0.4	6
42	Electronic and optical properties of C24, C12X6Y6, and X12Y12 (Xâ€‰=â€‰B, Al and Yâ€‰=â€‰N, P). Journal of Molecular Modeling, 2018, 24, 204.	1.8	25
43	Characterizing the sensitivity of bonds to the curvature of carbon nanotubes. Journal of Molecular Modeling, 2018, 24, 249.	1.8	25
44	Adsorption of Hydrazoic Acid on Pristine Graphyne Sheet: A Computational Study. Wuli Huaxue Xuebao/ Acta Physico - Chimica Sinica, 2018, 34, 537-542.	4.9	25
45	Unsymmetrical achiral four ring hockey stick shaped mesogens based on 1,3,4-oxadiazole: Photophysical, mesogenic and DFT studies. Journal of Molecular Liquids, 2017, 241, 881-896.	4.9	9
46	A first principle study of phosphorous doped graphyne. AIP Conference Proceedings, 2017, , .	0.4	3
47	Hockey-stick-shaped mesogens based on 1,3,4-thiadiazole: synthesis, mesomorphism, photophysical and DFT studies. Liquid Crystals, 2017, 44, 2203-2221.	2.2	31
48	Density functional theory study of pristine and transition metal doped fullerene. AIP Conference Proceedings, 2017, , .	0.4	16
49	Theoretical investigation of electronic, vibrational, and nonlinear optical properties of 4-fluoro-4-hydroxybenzophenone. Spectroscopy Letters, 2017, 50, 232-243.	1.0	41
50	Benzthiazoline-2-thione (BTT) revisited: An experimental and theoretical endeavor to understand UV-spectra. Chemical Physics Letters, 2017, 686, 88-96.	2.6	7
51	Electron transport property of tetrathiafulvalene molecule. AIP Conference Proceedings, 2016, , .	0.4	0
52	Electronic properties of aluminium and silicon doped (2, 2) graphyne nanotube. Journal of Physics: Conference Series, 2016, 759, 012038.	0.4	4
53	Confinement of water molecule inside (2, 2) graphyne nanotube. AIP Conference Proceedings, 2016, , .	0.4	8
54	Influence of polar substituent on central bending unit of bent core mesogens: Synthesis, photophysical, mesomorphism and DFT studies. Journal of Molecular Structure, 2016, 1119, 177-187.	3.6	3

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55	Tailored synthesis of CuS nanodisks from a new macrocyclic precursor and their efficient catalytic properties on methylene blue dye degradation. Journal of Nanoparticle Research, 2016, 18, 1.	1.9	13
56	First principle study of adsorption of boron-halogenated system on pristine graphyne. Structural Chemistry, 2016, 27, 1221-1227.	2.0	50
57	Graphyneâ€“graphene (nitride) heterostructure as nanocapacitor. Chemical Physics, 2016, 478, 73-80.	1.9	22
58	Interaction of nitrogen molecule with pristine and doped graphyne nanotube. Physica E: Low-Dimensional Systems and Nanostructures, 2016, 84, 330-339.	2.7	39
59	A computational study on structure, stability and bonding in Noble Gas bound metal Nitrates, Sulfates and Carbonates (Metal = Cu, Ag, Au). Journal of Chemical Sciences, 2016, 128, 1537-1548.	1.5	27
60	The Effect of Boron and Nitrogen Doping in Electronic, Magnetic, and Optical Properties of Graphyne. Journal of Physical Chemistry C, 2016, 120, 26793-26806.	3.1	94
61	Electronic Properties of Homo- and Heterobilayer Graphyne: The Idea of a Nanocapacitor. Journal of Physical Chemistry C, 2016, 120, 26579-26587.	3.1	57
62	Nickel cluster functionalised carbon nanotube for CO molecule detection: a theoretical study. Molecular Physics, 2016, 114, 671-680.	1.7	8
63	Electrical Property of Zigzag Graphene-Molecular Nanojunction. Advanced Science Letters, 2016, 22, 246-249.	0.2	1
64	Density Functional Study of Transition Metal Trapping on Graphene. Advanced Science Letters, 2016, 22, 208-211.	0.2	0
65	Electron transport property of cobalt-centered porphyrin-armchair graphene nanoribbon (AGNR) junction. AIP Conference Proceedings, 2015, , .	0.4	1
66	Tuning the magnetic property of vacancy-defected graphyne by transition metal absorption. AIP Conference Proceedings, 2015, , .	0.4	6
67	Pristine and <scp>BN</scp> doped graphyne derivatives for <scp>UV</scp> light protection. International Journal of Quantum Chemistry, 2015, 115, 820-829.	2.0	80
68	Reactivity dynamics of a confined molecule in presence of an external magnetic field. International Journal of Quantum Chemistry, 2015, 115, 144-157.	2.0	26
69	Electronic and optical properties of pristine and boronâ€“nitrogen doped graphyne nanotubes. Physical Chemistry Chemical Physics, 2015, 17, 19325-19341.	2.8	71
70	NO adsorption on nickel and nickelâ€“manganese bimetallic clusters: A density functional study. Physica E: Low-Dimensional Systems and Nanostructures, 2015, 73, 12-20.	2.7	9
71	Geometry, chemical reactivity and Raman spectra of gold clusters. Cogent Chemistry, 2015, 1, 1076713.	2.5	13
72	First principle study of sodium decorated graphyne. Chemical Physics, 2015, 461, 74-80.	1.9	34

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73	Emissive bis-salicylaldiminato Schiff base ligands and their zinc(II) complexes: Synthesis, photophysical properties, mesomorphism and DFT studies. Journal of Molecular Structure, 2015, 1081, 316-328.	3.6	29
74	Structure, vibrational, and optical properties of platinum cluster: a density functional theory approach. Journal of Molecular Modeling, 2014, 20, 2537.	1.8	32
75	Tuning of band gap due to fluorination of graphyne and graphdiyne. Journal of Physics: Conference Series, 2014, 566, 012014.	0.4	11
76	Reactivity dynamics of confined atoms in the presence of an external magnetic field. European Physical Journal D, 2014, 68, 1.	1.3	20
77	A density functional study of chemical, magnetic and thermodynamic properties of small palladium clusters. Molecular Simulation, 2014, 40, 1255-1264.	2.0	21
78	A first principle study of pristine and BN-doped graphyne family. Structural Chemistry, 2014, 25, 1695-1710.	2.0	84
79	Nickel Decorated Single-Wall Carbon Nanotube as CO Sensor. Soft Nanoscience Letters, 2013, 03, 9-11.	0.8	11
80	Interaction of Boron-Nitrogen Substitued Graphene Nanoribbon with Nucleobases: The Idea of Biosensor. Soft Nanoscience Letters, 2013, 03, 43-45.	0.8	3
81	A computational study of armchair nanotube. , 2012, , .		0
82	A tug-of-war between electronic excitation and confinement in a dynamical context. Physical Chemistry Chemical Physics, 2012, 14, 1716-1727.	2.8	40
83	Microstructure evolution of irradiated tungsten: Crystal effects in He and H implantation as modelled in the Binary Collision Approximation. Journal of Nuclear Materials, 2010, 403, 89-100.	2.7	36
84	Microstructural evolution of irradiated tungsten: Ab initio parameterisation of an OKMC model. Journal of Nuclear Materials, 2010, 403, 75-88.	2.7	177
85	Structure and thermodynamics of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Fe</mml:mtext></mml:mrow><mml:mrow><mml:mn>55</mml:mn xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Co</mml:mtext></mml:mrow><mml:mrow><mml:mn>55</mml:mn and<mml:math xmlns:mml="http://www.w3.org/1998/Math/. Physical Review B, 2009, 79, .	3.2	18
86	Moving least-squares enhanced Shepard interpolation for the fast marching and string methods. Journal of Chemical Physics, 2009, 130, 024103.	3.0	13
87	Dirichlet Boundary Conditions and Effect of Confinement on Chemical Reactivity. Journal of Physical Chemistry A, 2009, 113, 10759-10766.	2.5	32
88	Chapter 13 Chemical reactivity dynamics in ground and excited electronic states. Theoretical and Computational Chemistry, 2007, 19, 269-286.	0.4	10
89	Electronic Structure Principles and Aromaticity. Journal of Chemical Education, 2007, 84, 354.	2.3	68
90	Toxicity analysis of polychlorinated dibenzofurans through global and local electrophilicities. Computational and Theoretical Chemistry, 2006, 758, 119-125.	1.5	50

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91	Electrophilicity Index. Chemical Reviews, 2006, 106, 2065-2091.	47.7	1,383
92	Careful Scrutiny of the Philicity Concept. Journal of Physical Chemistry A, 2006, 110, 1084-1093.	2.5	87
93	Analyzing Toxicity Through Electrophilicity. Molecular Diversity, 2006, 10, 119-131.	3.9	115
94	Formaldehyde decomposition through profiles of global reactivity indices. Computational and Theoretical Chemistry, 2005, 723, 43-52.	1.5	41
95	Cracking of n-heptane in HZSM-5 zeolite. Computational and Theoretical Chemistry, 2005, 755, 99-103.	1.5	4
96	Relationship between electrophilicity index, Hammett constant and nucleus-independent chemical shift. Journal of Chemical Sciences, 2005, 117, 61-65.	1.5	29
97	A conceptual DFT approach towards analysing toxicity. Journal of Chemical Sciences, 2005, 117, 599-612.	1.5	36
98	DFT study of some aliphatic amines using generalized philicity concept. International Journal of Quantum Chemistry, 2005, 101, 690-702.	2.0	35
99	Effect of solvation on the condensed Fukui function and the generalized philicity index. Chemical Physics Letters, 2004, 383, 122-128.	2.6	80
100	Chemical reactivity of the compressed noble gas atoms and their reactivity dynamics during collisions with protons. Journal of Chemical Sciences, 2003, 115, 195-218.	1.5	11
101	Chemical reactivity of the spherically confined atoms. Chemical Physics Letters, 2003, 372, 805-809.	2.6	45
102	Ground- and excited-states reactivity dynamics of hydrogen and helium atoms. International Journal of Quantum Chemistry, 2003, 91, 633-650.	2.0	29
103	Effect of Spherical Confinement on Chemical Reactivity. Journal of Physical Chemistry A, 2003, 107, 4877-4882.	2.5	51
104	Philicity:Â A Unified Treatment of Chemical Reactivity and Selectivity. Journal of Physical Chemistry A, 2003, 107, 4973-4975.	2.5	660
105	A new N₂O₂-donor compartmental Schiff base ligand and its cadmium(II) complex: synthesis, mesogenic and photoluminescent properties. Inorganic and Nano-Metal Chemistry, 0, , 1-10.	1.6	0