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	Electrophilicity Index. Chemical Reviews, 2006, 106, 2065-2091.	47.7	1,383
2	Philicity:Â A Unified Treatment of Chemical Reactivity and Selectivity. Journal of Physical Chemistry A, 2003, 107, 4973-4975.	2.5	660
3	Microstructural evolution of irradiated tungsten: Ab initio parameterisation of an OKMC model. Journal of Nuclear Materials, 2010, 403, 75-88.	2.7	177
4	Analyzing Toxicity Through Electrophilicity. Molecular Diversity, 2006, 10, 119-131.	3.9	115
5	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
6	Careful Scrutiny of the Philicity Concept. Journal of Physical Chemistry A, 2006, 110, 1084-1093.	2.5	87
7	A first principle study of pristine and BN-doped graphyne family. Structural Chemistry, 2014, 25, 1695-1710.	2.0	84
8	MoS₂/MoO₃ Nanocomposite for Selective NH₃ Detection in a Humid Environment. ACS Sustainable Chemistry and Engineering, 2021, 9, 7328-7340.	6.7	84
9	Effect of solvation on the condensed Fukui function and the generalized philicity index. Chemical Physics Letters, 2004, 383, 122-128.	2.6	80
10	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
11	MoS₂/WO₃Nanosheets for Detection of Ammonia. ACS Applied Nano Materials, 2021, 4, 2594-2605.	5.0	80
12	MoSe₂ Crystalline Nanosheets for Room-Temperature Ammonia Sensing. ACS Applied Nano Materials, 2020, 3, 9375-9384.	5.0	79
13	Electronic and optical properties of pristine and boronâ€“nitrogen doped graphyne nanotubes. Physical Chemistry Chemical Physics, 2015, 17, 19325-19341.	2.8	71
14	Electronic Structure Principles and Aromaticity. Journal of Chemical Education, 2007, 84, 354.	2.3	68
15	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
16	Electronic Properties of Homo- and Heterobilayer Graphyne: The Idea of a Nanocapacitor. Journal of Physical Chemistry C, 2016, 120, 26579-26587.	3.1	57
17	Boron-nitride and boron-phosphide doped twin-graphene: Applications in electronics and optoelectronics. Applied Surface Science, 2021, 541, 148657.	6.1	53
18	Effect of Spherical Confinement on Chemical Reactivity. Journal of Physical Chemistry A, 2003, 107, 4877-4882.	2.5	51

#	ARTICLE	IF	CITATIONS
19	Toxicity analysis of polychlorinated dibenzofurans through global and local electrophilicities. Computational and Theoretical Chemistry, 2006, 758, 119-125.	1.5	50
20	First principle study of adsorption of boron-halogenated system on pristine graphyne. Structural Chemistry, 2016, 27, 1221-1227.	2.0	50
21	Ultrahigh carrier mobility of penta-graphene: A first-principle study. Physica E: Low-Dimensional Systems and Nanostructures, 2021, 127, 114507.	2.7	50
22	Pentagraphyne: a new carbon allotrope with superior electronic and optical property. Journal of Materials Chemistry C, 2020, 8, 16143-16150.	5.5	49
23	Chemical reactivity of the spherically confined atoms. Chemical Physics Letters, 2003, 372, 805-809.	2.6	45
24	Formaldehyde decomposition through profiles of global reactivity indices. Computational and Theoretical Chemistry, 2005, 723, 43-52.	1.5	41
25	Theoretical investigation of electronic, vibrational, and nonlinear optical properties of 4-fluoro-4-hydroxybenzophenone. Spectroscopy Letters, 2017, 50, 232-243.	1.0	41
26	A tug-of-war between electronic excitation and confinement in a dynamical context. Physical Chemistry Chemical Physics, 2012, 14, 1716-1727.	2.8	40
27	Interaction of nitrogen molecule with pristine and doped graphyne nanotube. Physica E: Low-Dimensional Systems and Nanostructures, 2016, 84, 330-339.	2.7	39
28	Twin-graphene as a Promising Anode Material for Na-Ion Rechargeable Batteries. ACS Applied Nano Materials, 2021, 4, 4912-4918.	5.0	39
29	A conceptual DFT approach towards analysing toxicity. Journal of Chemical Sciences, 2005, 117, 599-612.	1.5	36
30	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
31	DFT study of some aliphatic amines using generalized philicity concept. International Journal of Quantum Chemistry, 2005, 101, 690-702.	2.0	35
32	First principle study of sodium decorated graphyne. Chemical Physics, 2015, 461, 74-80.	1.9	34
33	Reactivity Dynamics. Journal of Physical Chemistry A, 2021, 125, 2051-2060.	2.5	34
34	Dirichlet Boundary Conditions and Effect of Confinement on Chemical Reactivity. Journal of Physical Chemistry A, 2009, 113, 10759-10766.	2.5	32
35	Structure, vibrational, and optical properties of platinum cluster: a density functional theory approach. Journal of Molecular Modeling, 2014, 20, 2537.	1.8	32
36	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

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37	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
38	Boron-phosphorous doped graphyne: A near-infrared light absorber. AIP Advances, 2019, 9, .	1.3	30
39	Ground- and excited-states reactivity dynamics of hydrogen and helium atoms. International Journal of Quantum Chemistry, 2003, 91, 633-650.	2.0	29
40	Relationship between electrophilicity index, Hammett constant and nucleus-independent chemical shift. Journal of Chemical Sciences, 2005, 117, 61-65.	1.5	29
41	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
42	MoSe2/multiwalled carbon nanotube composite for ammonia sensing in natural humid environment. Journal of Hazardous Materials, 2022, 435, 128821.	12.4	29
43	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
44	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
45	Detection of nitrobenzene using transition metal doped C24: A DFT study. Structural Chemistry, 2021, 32, 2259-2270.	2.0	26
46	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
47	Characterizing the sensitivity of bonds to the curvature of carbon nanotubes. Journal of Molecular Modeling, 2018, 24, 249.	1.8	25
48	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
49	Thermoelectric Properties of Pristine Graphyne and the BN-Doped Graphyne Family. ACS Omega, 2021, 6, 20149-20157.	3.5	24
50	Graphyneâ€“graphene (nitride) heterostructure as nanocapacitor. Chemical Physics, 2016, 478, 73-80.	1.9	22
51	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
52	A Detailed DFT Study on Electronic Structures and Nonlinear Optical Properties of Doped C₃₀. ChemistrySelect, 2020, 5, 6987-6999.	1.5	22
53	A density functional study of chemical, magnetic and thermodynamic properties of small palladium clusters. Molecular Simulation, 2014, 40, 1255-1264.	2.0	21
54	Raman and IR signature of pristine and BN- doped Î³-graphyne from first-principle. Carbon, 2019, 141, 652-662.	10.3	21

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55	Reactivity dynamics of confined atoms in the presence of an external magnetic field. European Physical Journal D, 2014, 68, 1.	1.3	20
56	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
57	Highly Selective Ethyl Mercaptan Sensing Using a MoSe₂/SnO₂ Composite at Room Temperature. ACS Applied Materials & Interfaces, 2022, 14, 23916-23927.	8.0	20
58	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
59	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
60	Density functional theory study of pristine and transition metal doped fullerene. AIP Conference Proceedings, 2017, , .	0.4	16
61	Designing nanoscale capacitors based on twin-graphene. Physical Chemistry Chemical Physics, 2021, 23, 16268-16276.	2.8	16
62	Moving least-squares enhanced Shepard interpolation for the fast marching and string methods. Journal of Chemical Physics, 2009, 130, 024103.	3.0	13
63	Geometry, chemical reactivity and Raman spectra of gold clusters. Cogent Chemistry, 2015, 1, 1076713.	2.5	13
64	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
65	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
66	High capacitance twinâ€graphene anode material for magnesium ion battery. Energy Storage, 2023, 5, .	4.3	13
67	Electronic, nonlinear optical and thermodynamic properties of (CdS) n clusters: A first principle study. Computational Condensed Matter, 2018, 14, 40-45.	2.1	12
68	Electronic and transport property of two-dimensional boron phosphide sheet. Journal of Molecular Graphics and Modelling, 2022, 112, 108117.	2.4	12
69	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
70	Tuning of band gap due to fluorination of graphyne and graphdiyne. Journal of Physics: Conference Series, 2014, 566, 012014.	0.4	11
71	The Influence of the Substitution of Transition Metals on Pristine C₂₀: A DFT Study. International Journal of Nanoscience, 2018, 17, 1760026.	0.7	11
72	Nickel Decorated Single-Wall Carbon Nanotube as CO Sensor. Soft Nanoscience Letters, 2013, 03, 9-11.	0.8	11

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73	Thermoelectric properties of pentagraphene. Physica B: Condensed Matter, 2022, 641, 414091.	2.7	11
74	Chapter 13 Chemical reactivity dynamics in ground and excited electronic states. Theoretical and Computational Chemistry, 2007, 19, 269-286.	0.4	10
75	Conceptual DFT based electronic structure principles in a dynamical context. Journal of the Indian Chemical Society, 2021, 98, 100098.	2.8	10
76	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
77	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
78	Confinement of water molecule inside (2, 2) graphyne nanotube. AIP Conference Proceedings, 2016, , .	0.4	8
79	Nickel cluster functionalised carbon nanotube for CO molecule detection: a theoretical study. Molecular Physics, 2016, 114, 671-680.	1.7	8
80	Donor-acceptor decorated graphyne: A promising candidate for nonlinear optical application. AIP Conference Proceedings, 2019, , .	0.4	8
81	Benzthiazoline-2-thione (BTT) revisited: An experimental and theoretical endeavor to understand UV-spectra. Chemical Physics Letters, 2017, 686, 88-96.	2.6	7
82	Tuning the magnetic property of vacancy-defected graphyne by transition metal absorption. AIP Conference Proceedings, 2015, , .	0.4	6
83	Transition metal doped (X = V, Cr) CdS monolayer: A DFT study. AIP Conference Proceedings, 2018, , .	0.4	6
84	Optical properties of C28 fullerene cage: A DFT study. AIP Conference Proceedings, 2018, , .	0.4	6
85	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
86	Theoretical study of electronic transport through P-porphyrin and S-porphyrin nanoribbons. Journal of Molecular Graphics and Modelling, 2020, 97, 107543.	2.4	5
87	Cracking of n-heptane in HZSM-5 zeolite. Computational and Theoretical Chemistry, 2005, 755, 99-103.	1.5	4
88	Electronic properties of aluminium and silicon doped (2, 2) graphyne nanotube. Journal of Physics: Conference Series, 2016, 759, 012038.	0.4	4
89	Influence of noble gas atoms on B12N12 fullerene: A DFT study. AIP Conference Proceedings, 2019, , .	0.4	4
90	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

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91	Low-temperature nematic phase in azo functionalised reactive hockey stick mesogens possessing lateral methyl group. Dyes and Pigments, 2020, 173, 107233.	3.7	4
92	Solvent Effects on the Photophysical Properties of a Donorâ€“acceptor Based Schiff Base. Journal of Fluorescence, 2022, 32, 1321-1336.	2.5	4
93	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
94	A first principle study of phosphorous doped graphyne. AIP Conference Proceedings, 2017, , .	0.4	3
95	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
96	Penta-BeS2 monolayer: A new 2D material. AIP Conference Proceedings, 2020, , .	0.4	3
97	Interaction of Boron-Nitrogen Substitued Graphene Nanoribbon with Nucleobases: The Idea of Biosensor. Soft Nanoscience Letters, 2013, 03, 43-45.	0.8	3
98	Electron transport property of cobalt-centered porphyrin-armchair graphene nanoribbon (AGNR) junction. AIP Conference Proceedings, 2015, , .	0.4	1
99	Tuning electronic properties of bilayer Î±2-graphyne by external electric field: a density functional theory study. Monatshefte FÃ¼r Chemie, 2021, 152, 61-66.	1.8	1
100	Electrical Property of Zigzag Graphene-Molecular Nanojunction. Advanced Science Letters, 2016, 22, 246-249.	0.2	1
101	A computational study of armchair nanotube. , 2012, , .		0
102	Electron transport property of tetrathiafulvalene molecule. AIP Conference Proceedings, 2016, , .	0.4	0
103	Density Functional Study of Transition Metal Trapping on Graphene. Advanced Science Letters, 2016, 22, 208-211.	0.2	0
104	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
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