Debesh R Roy

List of Publications by Year
in descending order

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106 papers	4,672 citations	159585 30 h-index	102487 66 g-index
107 all docs	107 docs citations	107 times ranked	3333 citing authors

#	Article	IF	Citations
1	Electrophilicity Index. Chemical Reviews, 2006, 106, 2065-2091.	47.7	1,383
2	Update 1 of: Electrophilicity Index. Chemical Reviews, 2007, 107, PR46-PR74.	47.7	509
3	Electrophilicity index as a possible descriptor of biological activity. Bioorganic and Medicinal Chemistry, 2004, 12, 5533-5543.	3.0	363
4	Electrophilicity as a possible descriptor for toxicity prediction. Bioorganic and Medicinal Chemistry, 2005, 13, 3405-3412.	3.0	173
5	Multiphilic Descriptor for Chemical Reactivity and Selectivity. Journal of Physical Chemistry A, 2007, 111, 9130-9138.	2.5	141
6	Analyzing Toxicity Through Electrophilicity. Molecular Diversity, 2006, 10, 119-131.	3.9	115
7	Local hardness: a critical account. Theoretical Chemistry Accounts, 2007, 118, 923-930.	1.4	95
8	Electronic and optical properties of BaTiO3 across tetragonal to cubic phase transition: An experimental and theoretical investigation. Journal of Applied Physics, 2017, 122, .	2.5	95
9	Stability and Reactivity of All-Metal Aromatic and Antiaromatic Systems in Light of the Principles of Maximum Hardness and Minimum Polarizability. Journal of Physical Chemistry A, 2005, 109, 9590-9597.	2.5	94
10	Careful Scrutiny of the Philicity Concept. Journal of Physical Chemistry A, 2006, 110, 1084-1093.	2.5	87
11	On the Ground State of Pd₁₃. Journal of the American Chemical Society, 2011, 133, 12192-12196.	13.7	74
12	Electronic Structure Principles and Aromaticity. Journal of Chemical Education, 2007, 84, 354.	2.3	68
13	Reactivity, Selectivity, and Aromaticity of Be₃²⁻ and Its Complexes. Journal of Physical Chemistry A, 2008, 112, 1612-1621.	2.5	57
14	Aromaticity in Polyacene Analogues of Inorganic Ring Compounds. Journal of Physical Chemistry A, 2007, 111, 4684-4696.	2.5	52
15	Single-layer stanane as potential gas sensor for NO2, SO2, CO2 and NH3 under DFT investigation. Physica E: Low-Dimensional Systems and Nanostructures, 2019, 110, 100-106.	2.7	48
16	Ca₂C MXene monolayer as a superior anode for metal-ion batteries. 2D Materials, 2021, 8, 035015.	4.4	44
17	Magnetic moment and local moment alignment in anionic and/or oxidized Fen clusters. Journal of Chemical Physics, 2010, 132, 194305.	3.0	41
18	Highly Sensitive Bifunctional Probe for Colorimetric Cyanide and Fluorometric H₂S Detection and Bioimaging: Spontaneous Resolution, Aggregation, and Multicolor Fluorescence of Bisulfide Adduct. Journal of Organic Chemistry, 2017, 82, 10234-10246.	3.2	40

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19	Two-Dimensional Boronâ€“Phosphorus Monolayer for Reversible NO₂ Gas Sensing. ACS Applied Nano Materials, 2020, 3, 10073-10081.	5.0	40
20	Chemical reactivity descriptor based aromaticity indices applied to and systems. Computational and Theoretical Chemistry, 2006, 759, 109-110.	1.5	39
21	An atom counting strategy towards analyzing the biological activity of sex hormones. European Journal of Medicinal Chemistry, 2007, 42, 1365-1369.	5.5	39
22	A conceptual DFT approach towards analysing toxicity. Journal of Chemical Sciences, 2005, 117, 599-612.	1.5	36
23	Optical activity of Co-porphyrin in the light of IR and Raman spectroscopy: A critical DFT investigation. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 190, 121-128.	3.9	36
24	Bonding, reactivity and aromaticity in the light of the multicenter indices. Computational and Theoretical Chemistry, 2008, 854, 35-39.	1.5	35
25	2D Sb2C3 monolayer: A promising material for the recyclable gas sensor for environmentally toxic nitrogen-containing gases (NCGs). Journal of Hazardous Materials, 2021, 405, 124168.	12.4	35
26	Exploiting unusual affinity of usual polysaccharides for separation of enzymes on fluidized beds. Enzyme and Microbial Technology, 2000, 27, 53-65.	3.2	34
27	An Electrophilicity Based Analysis of Toxicity of Aromatic Compounds TowardsTetrahymena Pyriformis. QSAR and Combinatorial Science, 2006, 25, 114-122.	1.4	32
28	Synthesis and structure of 1-D Na6cluster chain with short Naâ€“Na distance: Organic like aromaticity in inorganic metal cluster. Chemical Communications, 2007, , 135-137.	4.1	32
29	Are strong BrÃ¸nsted acids necessarily strong Lewis acids?. Computational and Theoretical Chemistry, 2007, 812, 13-24.	1.5	32
30	Local Descriptors around a Transition State:â€‰ A Link between Chemical Bonding and Reactivity. Journal of Physical Chemistry A, 2005, 109, 3771-3772.	2.5	31
31	Minimum magnetizability principle. Journal of Chemical Physics, 2006, 125, 056101.	3.0	31
32	Heterobilayer CaS/CaSe: A promising sensor for environmental toxic NO2 gas with high selectivity and sensitivity. Applied Surface Science, 2020, 528, 146996.	6.1	30
33	A Possible Union of Chemical Bonding, Reactivity, and Kinetics. Journal of Physical Chemistry A, 2006, 110, 11401-11403.	2.5	28
34	Bonding and aromaticity in an all-metal sandwich-like compound, <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.gif" display="inline" overflow="scroll"><mml:mrow><mml:msubsup><mml:mrow><mml:mtext>Be</mml:mtext></mml:mrow><mml:mrow><mml:mn>8</mml:mn></mml:mrow> Chemical Physics Letters, 2008, 460, 382-385.	2.6	28
35	Structure, bonding, stability, electronic, thermodynamic and thermoelectric properties of six different phases of indium nitride. Journal of Materials Science, 2018, 53, 8302-8313.	3.7	28
36	Bonding, aromaticity, and structure of trigonal dianion metal clusters. Journal of Computational Chemistry, 2010, 31, 1815-1821.	3.3	27

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37	Aromaticity in cyclic alkali clusters. Physical Chemistry Chemical Physics, 2008, 10, 2461.	2.8	26
38	Effect of Electronic and Geometric Shell Closures on the Stability of Neutral and Anionic TiNa_n (n = 1â^'13) Clusters. Journal of Physical Chemistry C, 2010, 114, 10739-10744.	3.1	26
39	The interaction of two-dimensional P2SiS nanosheet with environmental toxic NCG molecules for sensor application: A DFT study. Sensors and Actuators A: Physical, 2021, 322, 112608.	4.1	25
40	Monolayer PC3: A promising material for environmentally toxic nitrogen-containing multi gases. Journal of Hazardous Materials, 2022, 422, 126761.	12.4	25
41	Green synthesis of CuO nanoparticles using Azadirachta indica and its antibacterial activity for medicinal applications. Materials Research Express, 2018, 5, 095033.	1.6	24
42	Hydrogen-induced tunable electronic and optical properties of a two-dimensional penta-Pt₂N₄ monolayer. Physical Chemistry Chemical Physics, 2021, 23, 10409-10417.	2.8	24
43	A connection between softness and magnetizability. Computational and Theoretical Chemistry, 2007, 813, 63-65.	1.5	23
44	An atom counting and electrophilicity based QSTR approach. Journal of Chemical Sciences, 2007, 119, 475-488.	1.5	23
45	Monolayer Bi2C3: A promising sensor for environmentally toxic NCGs with high sensitivity and selectivity. Applied Surface Science, 2020, 534, 147609.	6.1	23
46	Electric field-induced band modulation of predicted ternary 2D MXC3 [M:XÂ= As:Ge, Sb:Sn and Bi:Pb] with strong stability and optical properties. Carbon, 2021, 172, 791-803.	10.3	21
47	First-Principles Calculations of SiBi Nanosheets as Sensors for Oxygen-Containing Gases. ACS Applied Nano Materials, 2021, 4, 2440-2451.	5.0	19
48	2D PC₃ as a promising thermoelectric material. Physical Chemistry Chemical Physics, 2020, 22, 8625-8632.	2.8	18
49	Structure, stability, electronic and thermoelectric properties of strontium chalcogenides. Physica E: Low-Dimensional Systems and Nanostructures, 2020, 119, 113965.	2.7	18
50	Electronic Structure Principles in Static and Dynamic Situations. Computing Letters, 2007, 3, 223-230.	0.5	16
51	An Atom Counting QSPR Protocol. QSAR and Combinatorial Science, 2008, 27, 208-230.	1.4	16
52	Structure investigation of CoxO y + (x=3â€“6, y=3â€“8) clusters by IR vibrational spectroscopy and DFT calculations. European Physical Journal D, 2014, 68, 1.	1.3	16
53	Arsenic toxicity: an atom counting and electrophilicity-based protocol. Molecular Diversity, 2009, 13, 551-556.	3.9	15
54	h-CaS and h-CaSe nanosheets in CaX (Xâ€‰=â€‰O, S, Se and Te) series: promising thermoelectric materials under DFT investigation. Applied Nanoscience (Switzerland), 2019, 9, 1845-1856.	3.1	15

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55	Zirconium-organic framework as a novel adsorbent for arsenate remediation from aqueous solutions. Journal of Molecular Liquids, 2022, 356, 118957.	4.9	15
56	Structural, electronic, vibrational, mechanical and thermoelectric properties of 2D and bulk BaX (X=O, S, Se and Te) series under DFT and BTE framework. Physica E: Low-Dimensional Systems and Nanostructures, 2021, 127, 114523.	2.7	13
57	Sc 3 N and Sc 2 C 2 encapsulated B 40 : Smarter than its carbon analogue. Physica E: Low-Dimensional Systems and Nanostructures, 2016, 84, 354-360.	2.7	12
58	Structure, electronic, optical and thermodynamic behavior on the polymerization of PMMA: A DFT investigation. Computational Biology and Chemistry, 2018, 72, 192-198.	2.3	12
59	Levofloxacin capped Ag-nanoparicles: A new highly selective sensor for cations under joint experimental and DFT investigation. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2017, 179, 178-187.	3.9	11
60	Hexagonal thallium nitride in (TlX) 2n+1 H 2n+4 [XÂ=ÂN, P, As; n Â=Â1â€“5] cluster series: A promising building motif for future smart nanomaterials. Materials Chemistry and Physics, 2017, 200, 368-375.	4.0	10
61	Strain-induced band modulation and excellent stability, transport and optical properties of penta-MP₂ (M = Ni, Pd, and Pt) monolayers. Nanoscale Advances, 2020, 2, 4566-4580.	4.6	10
62	A comparative DFT study on electronic, thermodynamic and optical properties of telluride compounds. Computational Materials Science, 2014, 88, 156-162.	3.0	9
63	DFT investigation on A4B4 (A=Cu, Ag; B=As, Sn) metalâ€“semiconductor alloy clusters for potential nanomaterials. Physica E: Low-Dimensional Systems and Nanostructures, 2015, 68, 224-231.	2.7	9
64	Green Synthesis of Triangular ZnO Nanoparticles Using Azadirachta indica Leaf Extract and Its Shape Dependency for Significant Antimicrobial Activity: Joint Experimental and Theoretical Investigation. Journal of Cluster Science, 2022, 33, 2517-2530.	3.3	9
65	Density functional investigation on hexagonal nanosheets and bulk thallium nitrides for possible thermoelectric applications. Applied Nanoscience (Switzerland), 2019, 9, 33-42.	3.1	8
66	Hybrid CaS/CaSe bilayer as a wide temperature range thermoelectric material. Physica E: Low-Dimensional Systems and Nanostructures, 2020, 119, 114014.	2.7	8
67	Green Synthesis of Dense Rock MgO Nanoparticles Using Carica Papaya Leaf Extract and its Shape Dependent Antimicrobial Activity: Joint Experimental and DFT Investigation. Journal of Cluster Science, 2022, 33, 1667-1675.	3.3	7
68	Two-Dimensional lithium fluoride (LiF) as an efficient hydrogen storage material. Applied Surface Science, 2022, 581, 151776.	6.1	7
69	Synthesis, characterization and significant antimicrobial properties of CZTS nanoparticles against pathogenic strains. Journal of the Indian Chemical Society, 2022, 99, 100351.	2.8	7
70	Theoretical study of microscopic solvation of NaOH in water: NaOH(H2O)n, n=1â€“10. Chemical Physics, 2012, 407, 92-96.	1.9	6
71	Toxicity prediction of PHDDs and phenols in the light of nucleic acid bases and DNA base pair interaction. Journal of Molecular Graphics and Modelling, 2015, 62, 128-137.	2.4	6
72	First principle investigation on 2D beryllium chalcogenides for thermoelectric and optical applications. Journal of Physics and Chemistry of Solids, 2022, 164, 110619.	4.0	6

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73	A DFT study on group III and V combined hexagonal clusters as potential building motifs for inorganic nanomaterials. Journal of Molecular Structure, 2012, 1007, 203-207.	3.6	5
74	Synthesis of Ciprofloxacin Drug Capped Silver Nanoparticles and Their Antimicrobial Activity: A Joint Spectrophotometric and Density Functional Investigation. Journal of Cluster Science, 2021, 32, 1575-1584.	3.3	5
75	Experimental and first-principles investigation on the structural, electronic and antimicrobial properties of nickel hydroxide nanoparticles. Journal of Physics and Chemistry of Solids, 2022, 160, 110367.	4.0	5
76	Electronic properties of hexagonal gallium phosphide: A DFT investigation. AIP Conference Proceedings, 2016, , .	0.4	4
77	Magnetic switching in Cr (xâ€¯=â€¯2â€“8) and its oxide cluster series. Journal of Magnetism and Magnetic Materials, 2018, 451, 32-37.	2.3	4
78	Structural, vibrational, electronic, elastic and thermoelectric properties of monolayer alkali halide compounds from first principles investigation. Materials Today Communications, 2021, 29, 102855.	1.9	4
79	Magic stability of Ga4Mg3 cluster in GaxMg3(x=1â€“6) series: A density functional study. Chemical Physics, 2013, 411, 6-10.	1.9	3
80	Structure, electronic properties, aromaticity and dynamics of M3N@C80 and M2C2@C82 (M=Sc, Y): A density functional study. Physica E: Low-Dimensional Systems and Nanostructures, 2015, 70, 157-164.	2.7	3
81	Electronic structure and optical properties of metal doped tetraphenylporphyrins. AIP Conference Proceedings, 2018, , .	0.4	3
82	Strain-induced electronic, stability and enhancement of thermoelectric performance of 2D Si2C3 monolayer: An emerging material for renewable energy. Physica E: Low-Dimensional Systems and Nanostructures, 2021, 132, 114769.	2.7	3
83	Magic Clusters in Si_xMg₃(x=1-10) Series: Potential Building Motifs for Inorganic Nanomaterials. Journal of Nano Research, 2013, 24, 77-84.	0.8	2
84	Bio-activity of aminosulfonyl ureas in the light of nucleic acid bases and DNA base pair interaction. Computational Biology and Chemistry, 2018, 75, 91-100.	2.3	2
85	Toxicity of polyhalogenated dibenzo-p-furans in the light of nucleic acid bases interaction. Computational Biology and Chemistry, 2018, 76, 225-231.	2.3	2
86	Biological activity of some ACAT inhibitors in the light of DFT-based quantum descriptors. Structural Chemistry, 2019, 30, 2379-2387.	2.0	2
87	Overview and Recent Advances in QSAR Studies. , 2016, , 29-60.		2
88	Modeling Ecotoxicity as Applied to some Selected Aromatic Compounds. , 0, , 1-24.		2
89	Group three nitride clusters as promising components for nanoelectronics. Materials Today Chemistry, 2022, 23, 100751.	3.5	2
90	Transverse electronic transport through nucleobase-pairs of a DNA wire. Materials Today Chemistry, 2022, 24, 100834.	3.5	2

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91	DFT investigation on structure, electronic and magnetic properties of Crn (n=2-8) clusters. AIP Conference Proceedings, 2016, , .	0.4	1
92	Structure, electronic and magnetic properties of Mnn (n=2-8) clusters: A DFT investigation. AIP Conference Proceedings, 2016, , .	0.4	1
93	2D and bulk h-MgSe materials from Mg Se (m, n= 1â€“3) clusters: Density functional investigation. Journal of Alloys and Compounds, 2016, 687, 130-134.	5.5	1
94	First principle study on the structure, electronic and optical properties of MoS2/AlN hybrid bilayer: A DFT investigation. AIP Conference Proceedings, 2017, , .	0.4	1
95	DFT investigation on the optical properties of 2D-CaSe. AIP Conference Proceedings, 2020, , .	0.4	1
96	Conceptual density functional theory and aromaticity. , 2021, , 285-319.		1
97	Aromaticity in alkali metal clusters: Role of the metalloligand and the size of the metal ion. Journal of Computational Methods in Sciences and Engineering, 2008, 7, 395-408.	0.2	0
98	Arsenic based hexagonal building motifs for inorganic nanomaterials. , 2014, , .		0
99	Tl4Mg3 in TlxMg3 (x = 1â€“6) series: A bimetallic magic cluster for novel cluster assembled nanomaterials. AIP Conference Proceedings, 2017, , .	0.4	0
100	DFT study on band gap tunability in boron doped monolayer SiC. AIP Conference Proceedings, 2018, , .	0.4	0
101	Synthesis and physicochemical characterizations and antimicrobial activity of ZnO nanoparticles. AIP Conference Proceedings, 2018, , .	0.4	0
102	Thermoelectric investigation on Mg3N2 monolayer. AIP Conference Proceedings, 2020, , .	0.4	0
103	First principle investigation on the optical properties of monolayer CaS. AIP Conference Proceedings, 2020, , .	0.4	0
104	Investigation on the thermoelectric properties of single & bilayers of SrS. AIP Conference Proceedings, 2020, , .	0.4	0
105	In4Mg3 in InxMg3 (x = 1 â€“ 6) series: a magic unit for future smart materials. Nanosystems: Physics, Chemistry, Mathematics, 2016, , 592-594.	0.4	0
106	Synthesis, Physicochemical Characterizations and Antimicrobial Activity of CuO Nanoparticles. Current Nanomaterials, 2018, 3, 121-125.	0.4	0