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	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
2	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
3	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
4	Monolayer PC3: A promising material for environmentally toxic nitrogen-containing multi gases. Journal of Hazardous Materials, 2022, 422, 126761.	12.4	25
5	Two-Dimensional lithium fluoride (LiF) as an efficient hydrogen storage material. Applied Surface Science, 2022, 581, 151776.	6.1	7
6	Group three nitride clusters as promising components for nanoelectronics. Materials Today Chemistry, 2022, 23, 100751.	3.5	2
7	Synthesis, characterization and significant antimicrobial properties of CZTS nanoparticles against pathogenic strains. Journal of the Indian Chemical Society, 2022, 99, 100351.	2.8	7
8	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
9	Zirconium-organic framework as a novel adsorbent for arsenate remediation from aqueous solutions. Journal of Molecular Liquids, 2022, 356, 118957.	4.9	15
10	Transverse electronic transport through nucleobase-pairs of a DNA wire. Materials Today Chemistry, 2022, 24, 100834.	3.5	2
11	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
12	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
13	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
14	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
15	Conceptual density functional theory and aromaticity. , 2021, , 285-319.		1
16	First-Principles Calculations of SiBi Nanosheets as Sensors for Oxygen-Containing Gases. ACS Applied Nano Materials, 2021, 4, 2440-2451.	5.0	19
17	Ca₂C MXene monolayer as a superior anode for metal-ion batteries. 2D Materials, 2021, 8, 035015.	4.4	44
18	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

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19	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
20	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
21	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
22	Thermoelectric investigation on Mg3N2 monolayer. AIP Conference Proceedings, 2020, , .	0.4	0
23	DFT investigation on the optical properties of 2D-CaSe. AIP Conference Proceedings, 2020, , .	0.4	1
24	Monolayer Bi2C3: A promising sensor for environmentally toxic NCGs with high sensitivity and selectivity. Applied Surface Science, 2020, 534, 147609.	6.1	23
25	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
26	Two-Dimensional Boronâ€“Phosphorus Monolayer for Reversible NO₂ Gas Sensing. ACS Applied Nano Materials, 2020, 3, 10073-10081.	5.0	40
27	First principle investigation on the optical properties of monolayer CaS. AIP Conference Proceedings, 2020, , .	0.4	0
28	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
29	2D PC₃ as a promising thermoelectric material. Physical Chemistry Chemical Physics, 2020, 22, 8625-8632.	2.8	18
30	Investigation on the thermoelectric properties of single & bilayers of SrS. AIP Conference Proceedings, 2020, , .	0.4	0
31	Hybrid CaS/CaSe bilayer as a wide temperature range thermoelectric material. Physica E: Low-Dimensional Systems and Nanostructures, 2020, 119, 114014.	2.7	8
32	Structure, stability, electronic and thermoelectric properties of strontium chalcogenides. Physica E: Low-Dimensional Systems and Nanostructures, 2020, 119, 113965.	2.7	18
33	Biological activity of some ACAT inhibitors in the light of DFT-based quantum descriptors. Structural Chemistry, 2019, 30, 2379-2387.	2.0	2
34	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
35	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
36	Density functional investigation on hexagonal nanosheets and bulk thallium nitrides for possible thermoelectric applications. Applied Nanoscience (Switzerland), 2019, 9, 33-42.	3.1	8

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37	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
38	DFT study on band gap tunability in boron doped monolayer SiC. AIP Conference Proceedings, 2018, , .	0.4	0
39	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
40	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
41	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
42	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
43	Synthesis and physicochemical characterizations and antimicrobial activity of ZnO nanoparticles. AIP Conference Proceedings, 2018, , .	0.4	0
44	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
45	Green synthesis of CuO nanoparticles using Azadirachta indica and its antibacterial activity for medicinal applications. Materials Research Express, 2018, 5, 095033.	1.6	24
46	Electronic structure and optical properties of metal doped tetraphenylporphyrins. AIP Conference Proceedings, 2018, , .	0.4	3
47	Synthesis, Physicochemical Characterizations and Antimicrobial Activity of CuO Nanoparticles. Current Nanomaterials, 2018, 3, 121-125.	0.4	0
48	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
49	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
50	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
51	Tl4Mg3 in TlxMg3 (x = 1â€“6) series: A bimetallic magic cluster for novel cluster assembled nanomaterials. AIP Conference Proceedings, 2017, , .	0.4	0
52	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
53	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
54	DFT investigation on structure, electronic and magnetic properties of Crn (n=2-8) clusters. AIP Conference Proceedings, 2016, , .	0.4	1

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55	Electronic properties of hexagonal gallium phosphide: A DFT investigation. AIP Conference Proceedings, 2016, , .	0.4	4
56	Structure, electronic and magnetic properties of Mnn (n=2-8) clusters: A DFT investigation. AIP Conference Proceedings, 2016, , .	0.4	1
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	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
59	Overview and Recent Advances in QSAR Studies. , 2016, , 29-60.		2
60	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
61	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
62	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
63	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
64	Arsenic based hexagonal building motifs for inorganic nanomaterials. , 2014, , .		0
65	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
66	A comparative DFT study on electronic, thermodynamic and optical properties of telluride compounds. Computational Materials Science, 2014, 88, 156-162.	3.0	9
67	Magic stability of Ga4Mg3 cluster in GaxMg3(x=1â€“6) series: A density functional study. Chemical Physics, 2013, 411, 6-10.	1.9	3
68	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
69	Theoretical study of microscopic solvation of NaOH in water: NaOH(H2O)n, n=1â€“10. Chemical Physics, 2012, 407, 92-96.	1.9	6
70	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
71	On the Ground State of Pd₁₃. Journal of the American Chemical Society, 2011, 133, 12192-12196.	13.7	74
72	Bonding, aromaticity, and structure of trigonal dianion metal clusters. Journal of Computational Chemistry, 2010, 31, 1815-1821.	3.3	27

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73	Magnetic moment and local moment alignment in anionic and/or oxidized Fen clusters. Journal of Chemical Physics, 2010, 132, 194305.	3.0	41
74	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
75	Arsenic toxicity: an atom counting and electrophilicity-based protocol. Molecular Diversity, 2009, 13, 551-556.	3.9	15
76	An Atom Counting QSPR Protocol. QSAR and Combinatorial Science, 2008, 27, 208-230.	1.4	16
77	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</ Chemical Physics Letters, 2008, 460, 382-385.	2.6	28
78	Bonding, reactivity and aromaticity in the light of the multicenter indices. Computational and Theoretical Chemistry, 2008, 854, 35-39.	1.5	35
79	Aromaticity in cyclic alkali clusters. Physical Chemistry Chemical Physics, 2008, 10, 2461.	2.8	26
80	Reactivity, Selectivity, and Aromaticity of Be₃²⁻ and Its Complexes. Journal of Physical Chemistry A, 2008, 112, 1612-1621.	2.5	57
81	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
82	Electronic Structure Principles in Static and Dynamic Situations. Computing Letters, 2007, 3, 223-230.	0.5	16
83	Update 1 of: Electrophilicity Index. Chemical Reviews, 2007, 107, PR46-PR74.	47.7	509
84	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
85	Aromaticity in Polyacene Analogues of Inorganic Ring Compounds. Journal of Physical Chemistry A, 2007, 111, 4684-4696.	2.5	52
86	Electronic Structure Principles and Aromaticity. Journal of Chemical Education, 2007, 84, 354.	2.3	68
87	Multiphilic Descriptor for Chemical Reactivity and Selectivity. Journal of Physical Chemistry A, 2007, 111, 9130-9138.	2.5	141
88	Are strong BrÃ¸nsted acids necessarily strong Lewis acids?. Computational and Theoretical Chemistry, 2007, 812, 13-24.	1.5	32
89	A connection between softness and magnetizability. Computational and Theoretical Chemistry, 2007, 813, 63-65.	1.5	23
90	An atom counting strategy towards analyzing the biological activity of sex hormones. European Journal of Medicinal Chemistry, 2007, 42, 1365-1369.	5.5	39

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91	Local hardness: a critical account. Theoretical Chemistry Accounts, 2007, 118, 923-930.	1.4	95
92	An atom counting and electrophilicity based QSTR approach. Journal of Chemical Sciences, 2007, 119, 475-488.	1.5	23
93	A Possible Union of Chemical Bonding, Reactivity, and Kinetics. Journal of Physical Chemistry A, 2006, 110, 11401-11403.	2.5	28
94	An Electrophilicity Based Analysis of Toxicity of Aromatic Compounds TowardsTetrahymena Pyriformis. QSAR and Combinatorial Science, 2006, 25, 114-122.	1.4	32
95	Chemical reactivity descriptor based aromaticity indices applied to and systems. Computational and Theoretical Chemistry, 2006, 759, 109-110.	1.5	39
96	Electrophilicity Index. Chemical Reviews, 2006, 106, 2065-2091.	47.7	1,383
97	Careful Scrutiny of the Philicity Concept. Journal of Physical Chemistry A, 2006, 110, 1084-1093.	2.5	87
98	Analyzing Toxicity Through Electrophilicity. Molecular Diversity, 2006, 10, 119-131.	3.9	115
99	Minimum magnetizability principle. Journal of Chemical Physics, 2006, 125, 056101.	3.0	31
100	Electrophilicity as a possible descriptor for toxicity prediction. Bioorganic and Medicinal Chemistry, 2005, 13, 3405-3412.	3.0	173
101	A conceptual DFT approach towards analysing toxicity. Journal of Chemical Sciences, 2005, 117, 599-612.	1.5	36
102	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
103	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
104	Electrophilicity index as a possible descriptor of biological activity. Bioorganic and Medicinal Chemistry, 2004, 12, 5533-5543.	3.0	363
105	Exploiting unusual affinity of usual polysaccharides for separation of enzymes on fluidized beds. Enzyme and Microbial Technology, 2000, 27, 53-65.	3.2	34
106	Modeling Ecotoxicity as Applied to some Selected Aromatic Compounds. , 0, , 1-24.		2