Chiranjib Majumder

List of Publications by Year
in descending order

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95	2,028	236925	276875
papers	citations	25 h-index	41 g-index

95	95	95	2276
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	A theoretical study on the interaction of aromatic amino acids with graphene and single walled carbon nanotube. Journal of Chemical Physics, 2009, 130, 124911.	3.0	251
2	Structure and bonding ofAu5M(M=Na, Mg, Al, Si, P, and S) clusters. Physical Review B, 2006, 74, .	3.2	113
3	Growth pattern and bonding trends in Pt (n= 2â€“13) clusters: Theoretical investigation based on first principle calculations. Chemical Physics Letters, 2007, 446, 374-379.	2.6	77
4	Structural and electronic properties ofAun(n=2â€“10)clusters and their interactions with single S atoms:Ab initiomolecular dynamics simulations. Physical Review B, 2006, 73, .	3.2	73
5	Alumina-supported sub-nanometer Pt₁₀ clusters: amorphization and role of the support material in a highly active CO oxidation catalyst. Journal of Materials Chemistry A, 2017, 5, 4923-4931.	10.3	72
6	Structural investigation of thiophene thiol adsorption on Au nanoclusters: Influence of back bonds. Journal of Chemical Physics, 2002, 117, 2819-2822.	3.0	58
7	Structural and electronic properties of Si[sub n], Si[sub n]+], and AlSi[sub nâ^'1] (n=2â€“13) clusters: Theoretical investigation based on ab initio molecular orbital theory. Journal of Chemical Physics, 2004, 121, 7756.	3.0	58
8	CO Oxidation by BNâ^'Fullerene Cage: Effect of Impurity on the Chemical Reactivity. ACS Nano, 2008, 2, 1422-1428.	14.6	56
9	Bimetallic Agâ€Pt Subâ€nanometer Supported Clusters as Highly Efficient and Robust Oxidation Catalysts. Angewandte Chemie - International Edition, 2018, 57, 1209-1213.	13.8	47
10	Structural and electronic properties of Sin, Sinâ^', and PSinâ^'1 clusters (2â©½nâ©½13): Theoretical investigation based on ab initio molecular orbital theory. Journal of Chemical Physics, 2006, 125, 074303.	3.0	46
11	Molecular Scale Rectifier:Â Theoretical Study. Journal of Physical Chemistry A, 2001, 105, 9454-9459.	2.5	45
12	Effect of Si adsorption on the atomic and electronic structure ofAunclusters(n=1â€“8)and the Au (111) surface: First-principles calculations. Physical Review B, 2007, 75, .	3.2	45
13	Impurity-doped Si10 cluster: Understanding the structural and electronic properties from first-principles calculations. Physical Review B, 2004, 70, .	3.2	43
14	Atomic and electronic structures of neutral and cationSnn(n=2â€“20)clusters: A comparative theoretical study with different exchange-correlation functionals. Physical Review B, 2005, 71, .	3.2	40
15	Atomic and electronic structures of neutral and charged Pbn clusters (n=2â€“15): Theoretical investigation based on density functional theory. Journal of Chemical Physics, 2007, 126, 244704.	3.0	40
16	Influence of Al substitution on the atomic and electronic structure of Si clusters by density functional theory and molecular dynamics simulations. Physical Review B, 2004, 69, .	3.2	39
17	Hydrogen storage on Ti decorated SiC nanostructures: A first principles study. International Journal of Hydrogen Energy, 2012, 37, 3733-3740.	7.1	39
18	Interactions of a conjugated molecular diode with small metal clusters of Cu, Ag, and Au: First-principles calculations. Journal of Chemical Physics, 2002, 117, 7669-7675.	3.0	38

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19	Evidence of a graphene-like Sn-sheet on a Au(111) substrate: electronic structure and transport properties from first principles calculations. Physical Chemistry Chemical Physics, 2015, 17, 6705-6712.	2.8	33
20	An insight into local environment of lanthanide ions in Sr₂SiO₄:Ln (Ln = Sm,) Tj ETQq0 0 0 rgBT /Overlock 10	2.8	32
21	Structure and electronic properties of PbnM (M=C, Al, In, Mg, Sr, Ba, and Pb; n=8, 10, 12, and 14) clusters: Theoretical investigations based on first principles calculations. Journal of Chemical Physics, 2008, 128, 024308.	3.0	31
22	Fragmentation of small tin cluster ions (Snx+: x=4â€“20) in the low-energy collisions with a highly oriented pyrolytic graphite surface. Journal of Chemical Physics, 2002, 117, 4317-4322.	3.0	29
23	Growth Pattern of Ag_n(n= 1â^’8) Clusters on the Î±-Al₂O₃(0001) Surface: A First Principles Study. Langmuir, 2010, 26, 18776-18787.	3.5	27
24	Room temperature ammonia sensor based on jaw like bis-porphyrin molecules. Organic Electronics, 2013, 14, 1189-1196.	2.6	26
25	Enhancement of dielectric constant in a niobium doped titania system: an experimental and theoretical study. New Journal of Chemistry, 2016, 40, 9526-9536.	2.8	26
26	Thiophene thiol on the Au(111) surface: Size-dependent adsorption study. Journal of Chemical Physics, 2003, 118, 9809-9813.	3.0	25
27	Single atom alloy catalyst for SO₃ decomposition: enhancement of platinum catalyst's performance by Ag atom embedding. Nanoscale, 2018, 10, 20599-20610.	5.6	24
28	Energy level reordering and stability of MPb12 clusters: An interplay between geometry and electronic structure. Chemical Physics Letters, 2006, 430, 101-107.	2.6	23
29	Effect of substituent groups on the electronic properties of a molecular device: an ab initio theoretical study. Computational and Theoretical Chemistry, 2004, 681, 65-69.	1.5	21
30	Structure and bonding of tetramer clusters: Theoretical understanding of the aromaticity. Computational and Theoretical Chemistry, 2005, 755, 187-194.	1.5	21
31	Theoretical study of aromaticity in inorganic tetramer clusters. Journal of Chemical Sciences, 2006, 118, 575-578.	1.5	21
32	Molecular Resistance in a Molecular Diode:Â A Case Study of the Substituted Phenylethynyl Oligomer. Journal of Physical Chemistry A, 2002, 106, 7911-7914.	2.5	20
33	Oxidation of Al doped Au clusters: A first principles study. Journal of Chemical Physics, 2009, 130, 234309.	3.0	20
34	Adsorption of Small Palladium Clusters on the Î±-Al₂O₃(0001) Surface: A First Principles Study. Journal of Physical Chemistry C, 2012, 116, 2863-2871.	3.1	20
35	Adsorption of Thiols on the Pd(111) Surface: A First Principles Study. Langmuir, 2008, 24, 10838-10842.	3.5	18
36	A novel design for porphyrin based Dâ€“sâ€“A systems as molecular rectifiers. Chemical Science, 2016, 7, 1548-1557.	7.4	18

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37	Ionization potentials of small tin clusters: first principles calculations. Chemical Physics Letters, 2002, 356, 36-42.	2.6	17
38	Growth pattern and electronic properties of acetonitrile clusters: A density functional study. Journal of Chemical Physics, 2008, 128, 214307.	3.0	17
39	First-principles calculations to investigate electronic structure and transport properties of CrC monolayers: A new horizon for spintronic application. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 2021, 272, 115379.	3.5	17
40	Theoretical study of the alkyl derivative C 37 H 50 N 4 O 4 molecule for use as a stable molecular rectifier: geometric and electronic structures. Computational Materials Science, 2003, 27, 161-165.	3.0	15
41	ORR viability of alumina-supported platinum nanocluster: exploring oxidation behaviour by DFT. Physical Chemistry Chemical Physics, 2017, 19, 19308-19315.	2.8	15
42	The structural and electronic properties of Au_nclusters on the Î±-Al₂O₃(0001) surface: a first principles study. Physical Chemistry Chemical Physics, 2014, 16, 26561-26569.	2.8	14
43	Half metallicity and ferromagnetism of vanadium nitride nanoribbons: a first-principles study. Physical Chemistry Chemical Physics, 2021, 23, 1127-1138.	2.8	14
44	Chair like NiAu6: Clusters assemblies and CO oxidation study by ab initio methods. Chemical Physics Letters, 2013, 584, 108-112.	2.6	13
45	Do Agn (up to n = 8) clusters retain their identity on graphite? Insights from first-principles calculations including dispersion interactions. Journal of Chemical Physics, 2014, 140, 164705.	3.0	13
46	Magnetic needles encapsulated inside (BN)36 cage: Prediction of atomic, electronic, and magnetic structure from first principle calculations. Applied Physics Letters, 2007, 91, 223112.	3.3	12
47	M atom (M = Cu, Ag and Au) interaction with Ag and Au substrates: a first-principles study using cluster and slab models. Journal of Physics Condensed Matter, 2010, 22, 435001.	1.8	12
48	Silicon-pyrene/perylene hybrids as molecular rectifiers. Physical Chemistry Chemical Physics, 2015, 17, 1891-1899.	2.8	12
49	Impact of van der Waalâ€™s interaction in the hybrid bilayer of silicene/SiC. RSC Advances, 2016, 6, 21948-21953.	3.6	11
50	Microscopic Insights into Hydrogen Permeation Through a Model PdCu Membrane from First-Principles Investigations. Journal of Physical Chemistry C, 2018, 122, 12920-12933.	3.1	11
51	Are Deposited Bimetallic Clusters More Effective for SO₃ Decomposition? A Systematic Study Using First Principles Theory. Journal of Physical Chemistry C, 2012, 116, 25594-25601.	3.1	10
52	Influence of U doping on the growth behavior, electronic structure and magnetic properties of Pd n (n = 1â€“12) clusters: a first principles study. European Physical Journal D, 2014, 68, 1.	1.3	10
53	The nonchalant magnetic ordering of vacancies in graphene. Carbon, 2015, 91, 358-369.	10.3	10
54	Stability and electronic properties of Au atom doped hexagonal boron nitride sheet on Ni(111) support: Role of vacancy defects and supports towards single atom catalysis. Applied Surface Science, 2020, 515, 145978.	6.1	10

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55	Stabilizing Co, Ni and Cu on the h-BN surface: Using O O bond activation to probe their performance as single atom catalyst. Catalysis Today, 2021, 370, 75-82.	4.4	10
56	Theoretical Analysis for a Molecular Resonant Tunneling Diode. Japanese Journal of Applied Physics, 2002, 41, 2770-2773.	1.5	9
57	Influence of Sn interaction on the structural evolution of Au clusters: A first principles study. Chemical Physics Letters, 2012, 543, 121-126.	2.6	9
58	Conformers of hydrogenated SiC honeycomb structure: A first principles study. AIP Advances, 2013, 3, 082136.	1.3	9
59	Adsorption and decomposition of dimethyl methylphosphonate on pristine and mono-vacancy defected graphene: A first principles study. Applied Surface Science, 2017, 418, 318-327.	6.1	9
60	Molecular orbital analysis of frontier orbitals for molecular electronics: a case study of unimolecular rectifier and photovoltaic cell. Science and Technology of Advanced Materials, 2003, 4, 377-382.	6.1	8
61	Substrate induced reconstruction and activation of platinum clusters: A systematic DFT study. Applied Surface Science, 2017, 422, 1075-1081.	6.1	8
62	Experimental and theoretical investigation of the high dielectric permittivity of tantalum doped titania. New Journal of Chemistry, 2017, 41, 13067-13075.	2.8	8
63	Stable negative differential resistance in porphyrin based Ïƒâ€“Ï€â€“Ïƒ monolayers grafted on silicon. RSC Advances, 2015, 5, 50234-50244.	3.6	7
64	Size induced modification of boron structural unit in YBO₃: systematic investigation by experimental and theoretical methods. RSC Advances, 2016, 6, 64065-64071.	3.6	7
65	Atomically precise noble metal clusters (Ag10, Au10, Pd10 and Pt10) on alumina support: A comprehensive DFT study for oxidative catalysis. Applied Surface Science, 2021, 547, 149160.	6.1	7
66	Microsolvation of sodium ion in acetonitrile clusters: Structure and energetic trend by first principle study. Computational and Theoretical Chemistry, 2009, 907, 22-28.	1.5	6
67	A first principle study of SO3 decomposition on silver nano-clusters: Implications toward hydrogen production. International Journal of Hydrogen Energy, 2012, 37, 3645-3651.	7.1	6
68	Structural and electronic properties of Agâ€“Pd bimetallic clusters on Al2O3 substrates: A first principles study. Chemical Physics Letters, 2012, 537, 69-74.	2.6	6
69	Tuning of electron tunneling: a case study using BODIPY molecular layers. Physical Chemistry Chemical Physics, 2020, 22, 2098-2104.	2.8	6
70	Revisiting galvanic replacement between silver nanoparticles and mercury(II) ions in a cellulose membrane intended for optical assay application: Some new insights into silver-mercury interaction. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2020, 602, 125140.	4.7	6
71	Multiphoton dissociation/ionisation of dimethyl sulphide (CH3SCH3) at 355 and 532 nm. Journal of Chemical Sciences, 2001, 113, 129-138.	1.5	5
72	Stable fcc cage of III-IV mixed clusters with large energy gaps: Predictions based onab initiomolecular dynamics simulations. Physical Review B, 2004, 70, .	3.2	5

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73	Diffusion of Cd and Te adatoms on CdTe(111) surfaces: A computational study using density functional theory. AIP Advances, 2015, 5, .	1.3	5
74	Bipyridinium Molecular Switch: <I>Ab-initio</I> Electronic Structure Calculation. Materials Transactions, 2001, 42, 2276-2278.	1.2	4
75	Comparison between cluster and slab model for Pt-group atom adsorption on gold and silver substrate. Surface Science, 2014, 630, 78-84.	1.9	4
76	Platinum-Mediated Activation of Coordinated Organonitriles by Telluroethers in Tetrahydrofuran: Isolation, Structural Characterization, and Density Functional Theory Analysis of Intermediate Complexes. Inorganic Chemistry, 2015, 54, 11741-11750.	4.0	4
77	Is mixed oxide of Sn x Ti 1â^'x O 2 more effective for H 2 O decomposition? A first principles study. Chemical Physics Letters, 2015, 633, 175-180.	2.6	4
78	Intermolecular Aurophilic versus Intramolecular Auâ‹…â‹…â‹…N Secondary Interactions in Twoâ€Coordinate Gold(I) Selenolate Complexes. ChemistrySelect, 2016, 1, 4131-4136.	1.5	4
79	Probing Kinetics and Mechanism of Formation of Mixed Metallic Nanoparticles in a Polymer Membrane by Galvanic Replacement between Two Immiscible Metals: Case Study of Nickel/Silver Nanoparticle Synthesis. Langmuir, 2021, 37, 1637-1650.	3.5	4
80	Oxidation of tin clusters: A first principles study. Chemical Physics Letters, 2011, 518, 70-75.	2.6	3
81	Bimetallic Agâ€Pt Subâ€nanometer Supported Clusters as Highly Efficient and Robust Oxidation Catalysts. Angewandte Chemie, 2018, 130, 1223-1227.	2.0	3
82	Charge reordering of MgO (1Â0Â0) surface by Sn cluster deposition: Implications for heterogeneous catalysis. Applied Surface Science, 2020, 506, 144963.	6.1	3
83	Theoretical study of pure (Sin) and doped silicon (AlSin-1 and PSin-1) clusters (n=2â€“13) using ab initio molecular orbital theory. Journal of Computational Methods in Sciences and Engineering, 2008, 7, 319-335.	0.2	2
84	Activation of hydrogen iodide on silver tetramers: Role of confinement. Chemical Physics Letters, 2018, 705, 71-77.	2.6	2
85	Adsorption behavior of diatomic gases with defected hexagonal boron nitride nanosheet: A DFT study. Materials Today Communications, 2022, 31, 103813.	1.9	2
86	Structural Dependence of Magnetic Shielding Properties in Al₄Li₄ Clusters. Materials Transactions, 2008, 49, 2429-2436.	1.2	1
87	Adsorption of Eu atom at the TiO[sub 2] anatase (101) and rutile (110) surfaces. , 2013, , .		1
88	Role of size, composition and substrate in controlling the reactivity of Î±(0001)-Al 2 O 3 supported Ag n Au m (n+m = 2 â^' 4) alloy clusters for CO-oxidation: A comprehensive density functional study. Applied Surface Science, 2018, 433, 756-764.	6.1	1
89	Interaction of ammonia with semiconducting oxide surfaces. AIP Conference Proceedings, 2018, , .	0.4	1
90	First principles investigation of growth of small Pd-Ga bimetallic clusters on MgO(100) surface. Journal of Applied Physics, 2019, 125, .	2.5	1

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91	Study of Silicon-metal Interaction in Adsorption Process: An Ab-initio Approach. Materials Research Society Symposia Proceedings, 2011, 1305, 1.	0.1	0
92	Platinum atomic wire encapsulated in gold nanotubes: A first principle study. , 2014, , .		0
93	Catalytic behavior of â€˜Pt-atomic chain encapsulated gold nanotubeâ€™: A density functional study. AIP Conference Proceedings, 2016, , .	0.4	0
94	Oxidation of Sn doped Cu cluster: A first principle study. AIP Conference Proceedings, 2017, , .	0.4	0
95	Structural and electronic properties of Sn substituted Cun (n=10, 13) clusters: A first principles study. AIP Conference Proceedings, 2017, , .	0.4	0