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	Adsorption behavior of diatomic gases with defected hexagonal boron nitride nanosheet: A DFT study. Materials Today Communications, 2022, 31, 103813.	1.9	2
2	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
3	Half metallicity and ferromagnetism of vanadium nitride nanoribbons: a first-principles study. Physical Chemistry Chemical Physics, 2021, 23, 1127-1138.	2.8	14
4	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
5	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
6	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
7	Tuning of electron tunneling: a case study using BODIPY molecular layers. Physical Chemistry Chemical Physics, 2020, 22, 2098-2104.	2.8	6
8	Charge reordering of MgO (1ÂÔÂ0) surface by Sn cluster deposition: Implications for heterogeneous catalysis. Applied Surface Science, 2020, 506, 144963.	6.1	3
9	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
10	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
11	First principles investigation of growth of small Pd-Ga bimetallic clusters on MgO(100) surface. Journal of Applied Physics, 2019, 125, .	2.5	1
12	Bimetallic Agâ€Pt Subâ€nanometer Supported Clusters as Highly Efficient and Robust Oxidation Catalysts. Angewandte Chemie, 2018, 130, 1223-1227.	2.0	3
13	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
14	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
15	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
16	Activation of hydrogen iodide on silver tetramers: Role of confinement. Chemical Physics Letters, 2018, 705, 71-77.	2.6	2
17	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
18	Interaction of ammonia with semiconducting oxide surfaces. AIP Conference Proceedings, 2018, , .	0.4	1

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19	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
20	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
21	Substrate induced reconstruction and activation of platinum clusters: A systematic DFT study. Applied Surface Science, 2017, 422, 1075-1081.	6.1	8
22	Experimental and theoretical investigation of the high dielectric permittivity of tantalum doped titania. New Journal of Chemistry, 2017, 41, 13067-13075.	2.8	8
23	Oxidation of Sn doped Cu cluster: A first principle study. AIP Conference Proceedings, 2017, , .	0.4	0
24	Structural and electronic properties of Sn substituted Cun (n=10, 13) clusters: A first principles study. AIP Conference Proceedings, 2017, , .	0.4	0
25	ORR viability of alumina-supported platinum nanocluster: exploring oxidation behaviour by DFT. Physical Chemistry Chemical Physics, 2017, 19, 19308-19315.	2.8	15
26	Catalytic behavior of â€˜Pt-atomic chain encapsulated gold nanotubeâ€™: A density functional study. AIP Conference Proceedings, 2016, , .	0.4	0
27	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
28	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
29	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
30	Impact of van der Waalâ€™s interaction in the hybrid bilayer of silicene/SiC. RSC Advances, 2016, 6, 21948-21953.	3.6	11
31	A novel design for porphyrin based Dâ€“sâ€“A systems as molecular rectifiers. Chemical Science, 2016, 7, 1548-1557.	7.4	18
32	The nonchalant magnetic ordering of vacancies in graphene. Carbon, 2015, 91, 358-369.	10.3	10
33	Stable negative differential resistance in porphyrin based Ïƒâ€“Ï€â€“Ïƒ monolayers grafted on silicon. RSC Advances, 2015, 5, 50234-50244.	3.6	7
34	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
35	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
36	An insight into local environment of lanthanide ions in Sr₂SiO₄:Ln (Ln = Sm,) Tj ETQq0 0 0 rgBT /Overlock 10	2.8	32

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37	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
38	Diffusion of Cd and Te adatoms on CdTe(111) surfaces: A computational study using density functional theory. AIP Advances, 2015, 5, .	1.3	5
39	Silicon-pyrene/perylene hybrids as molecular rectifiers. Physical Chemistry Chemical Physics, 2015, 17, 1891-1899.	2.8	12
40	Platinum atomic wire encapsulated in gold nanotubes: A first principle study. , 2014, , .		0
41	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
42	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
43	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
44	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
45	Conformers of hydrogenated SiC honeycomb structure: A first principles study. AIP Advances, 2013, 3, 082136.	1.3	9
46	Room temperature ammonia sensor based on jaw like bis-porphyrin molecules. Organic Electronics, 2013, 14, 1189-1196.	2.6	26
47	Chair like NiAu6: Clusters assemblies and CO oxidation study by ab initio methods. Chemical Physics Letters, 2013, 584, 108-112.	2.6	13
48	Adsorption of Eu atom at the TiO[sub 2] anatase (101) and rutile (110) surfaces. , 2013, , .		1
49	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
50	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
51	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
52	Hydrogen storage on Ti decorated SiC nanostructures: A first principles study. International Journal of Hydrogen Energy, 2012, 37, 3733-3740.	7.1	39
53	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
54	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

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55	Oxidation of tin clusters: A first principles study. Chemical Physics Letters, 2011, 518, 70-75.	2.6	3
56	Study of Silicon-metal Interaction in Adsorption Process: An Ab-initio Approach. Materials Research Society Symposia Proceedings, 2011, 1305, 1.	0.1	0
57	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
58	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
59	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
60	Oxidation of Al doped Au clusters: A first principles study. Journal of Chemical Physics, 2009, 130, 234309.	3.0	20
61	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
62	Adsorption of Thiols on the Pd(111) Surface: A First Principles Study. Langmuir, 2008, 24, 10838-10842.	3.5	18
63	CO Oxidation by BNâ^'Fullerene Cage: Effect of Impurity on the Chemical Reactivity. ACS Nano, 2008, 2, 1422-1428.	14.6	56
64	Growth pattern and electronic properties of acetonitrile clusters: A density functional study. Journal of Chemical Physics, 2008, 128, 214307.	3.0	17
65	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
66	Structural Dependence of Magnetic Shielding Properties in Al₄Li₄ Clusters. Materials Transactions, 2008, 49, 2429-2436.	1.2	1
67	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
68	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
69	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
70	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
71	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
72	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

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73	Structure and bonding ofAu5M(M=Na, Mg, Al, Si, P, and S) clusters. Physical Review B, 2006, 74, .	3.2	113
74	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
75	Theoretical study of aromaticity in inorganic tetramer clusters. Journal of Chemical Sciences, 2006, 118, 575-578.	1.5	21
76	Structural and electronic properties of Sin, Sinâˆ', and PSinâˆ'1 clusters (2â©½nâ©½13): Theoretical investigation based on ab initio molecular orbital theory. Journal of Chemical Physics, 2006, 125, 074303.	3.0	46
77	Structure and bonding of tetramer clusters: Theoretical understanding of the aromaticity. Computational and Theoretical Chemistry, 2005, 755, 187-194.	1.5	21
78	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
79	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
80	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
81	Structural and electronic properties of Si[sub n], Si[sub n]+], and AlSi[sub nâˆ'1] (n=2â€“13) clusters: Theoretical investigation based on ab initio molecular orbital theory. Journal of Chemical Physics, 2004, 121, 7756.	3.0	58
82	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
83	Impurity-doped Si10 cluster: Understanding the structural and electronic properties from first-principles calculations. Physical Review B, 2004, 70, .	3.2	43
84	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
85	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
86	Thiophene thiol on the Au(111) surface: Size-dependent adsorption study. Journal of Chemical Physics, 2003, 118, 9809-9813.	3.0	25
87	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
88	Structural investigation of thiophene thiol adsorption on Au nanoclusters: Influence of back bonds. Journal of Chemical Physics, 2002, 117, 2819-2822.	3.0	58
89	Theoretical Analysis for a Molecular Resonant Tunneling Diode. Japanese Journal of Applied Physics, 2002, 41, 2770-2773.	1.5	9
90	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

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91	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
92	Ionization potentials of small tin clusters: first principles calculations. Chemical Physics Letters, 2002, 356, 36-42.	2.6	17
93	Bipyridinium Molecular Switch: <I>Ab-initio</I> Electronic Structure Calculation. Materials Transactions, 2001, 42, 2276-2278.	1.2	4
94	Multiphoton dissociation/ionisation of dimethyl sulphide (CH3SCH3) at 355 and 532 nm. Journal of Chemical Sciences, 2001, 113, 129-138.	1.5	5
95	Molecular Scale Rectifier:Â Theoretical Study. Journal of Physical Chemistry A, 2001, 105, 9454-9459.	2.5	45