Pranab Sarkar

List of Publications by Year
in descending order

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147 papers	2,846 citations	172207 29 h-index	264894 42 g-index
147 all docs	147 docs citations	147 times ranked	2775 citing authors

#	Article	IF	Citations
1	Polaron Induced Conductance Switching in Conjugated Oligophenylene: A First-Principles Analysis. Journal of Physical Chemistry A, 2022, 126, 318-324.	1.1	1
2	Rational Design of Two-Dimensional Porous Boron Phosphide as Efficient Cathode Material for Li and Na Ion Batteries: A First-Principles Study. Journal of Physical Chemistry C, 2022, 126, 5092-5100.	1.5	24
3	2D Homogeneous Holey Carbon Nitride: An Efficient Anode Material for Liâ€ion Batteries With Ultrahigh Capacity. ChemPhysChem, 2022, 23, .	1.0	12
4	2D lead free Ruddlesden-Popper phase perovskites as efficient photovoltaic materials: A first-principles investigation. Computational Materials Science, 2022, 211, 111545.	1.4	6
5	Towards H₂O catalyzed N₂-fixation over TiO₂ doped Ru_n clusters (n = 5, 6): a mechanistic and kinetic approach. Physical Chemistry Chemical Physics, 2021, 23, 1527-1538.	1.3	17
6	Half metallicity and ferromagnetism of vanadium nitride nanoribbons: a first-principles study. Physical Chemistry Chemical Physics, 2021, 23, 1127-1138.	1.3	14
7	Conductance switching of a gold-covalent organic framework nanojunction via proton transfer. Physics Letters, Section A: General, Atomic and Solid State Physics, 2021, 389, 127100.	0.9	2
8	Tuning the structural skeleton of a phenanthroline-based covalent organic framework for better electrochemical performance as a cathode material for Zn-ion batteries: a theoretical exploration. Physical Chemistry Chemical Physics, 2021, 23, 12644-12653.	1.3	19
9	Graphitic Carbon Nitride Sheet Supported Single-Atom Metal-Free Photocatalyst for Oxygen Reduction Reaction: A First-Principles Analysis. Journal of Physical Chemistry Letters, 2021, 12, 2788-2795.	2.1	38
10	Common Defects Accelerate Charge Separation and Reduce Recombination in CNT/Molecule Composites: Atomistic Quantum Dynamics. Journal of the American Chemical Society, 2021, 143, 6649-6656.	6.6	35
11	Photo-redox coupled Co-pincer complexes for efficient decarbonylation of aryl carbonyls: A quantum chemical investigation. Molecular Catalysis, 2021, 507, 111553.	1.0	2
12	Encapsulation and Stabilization of a Donorâ€“Acceptor Stenhouse Adduct Isomer in Water Inside the Blue Box: A Combined Experimental and Theoretical Approach. Journal of Physical Chemistry B, 2021, 125, 7222-7230.	1.2	2
13	Arene and functionalized arene based two dimensional <scp>organicâ€“inorganic</scp> hybrid perovskites for photovoltaic applications. Journal of Computational Chemistry, 2021, 42, 1982-1990.	1.5	16
14	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.	1.7	17
15	Lead Free Two-Dimensional Mixed Tin and Germanium Halide Perovskites for Photovoltaic Applications. Journal of Physical Chemistry C, 2021, 125, 74-81.	1.5	29
16	Dual-Silicon-Doped Graphitic Carbon Nitride Sheet: An Efficient Metal-Free Electrocatalyst for Urea Synthesis. Journal of Physical Chemistry Letters, 2021, 12, 10837-10844.	2.1	40
17	Molybdenum Atom-Mediated Salphen-Based Covalent Organic Framework as a Promising Electrocatalyst for the Nitrogen Reduction Reaction: A First-Principles Study. Journal of Physical Chemistry C, 2021, 125, 26061-26072.	1.5	34
18	Bis(iminothiolato)-Based One-Dimensional Metalâ€“Organic Framework: Robust Bipolar Magnetic Semiconductor with Reversal of Spin Polarization. Journal of Physical Chemistry C, 2020, 124, 37-43.	1.5	14

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19	Tunable Electronic Structure of Two-Dimensional MoX₂ (X = S, Se)/SnS₂ van der Waals Heterostructures. Journal of Physical Chemistry C, 2020, 124, 21357-21365.	1.5	16
20	Two-dimensional <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">CP</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math> monolayer and its fluorinated derivative with promising electronic and optical properties: A theoretical study. Physical Review B, 2020, 101, .	1.1	27
21	Highly Efficient Inorganicâ€“Organic Heterojunction Solar Cells Based on Polymer and CdX (X = Se, Te) Quantum Dots: An Insight from a Theoretical Study. Journal of Physical Chemistry C, 2020, 124, 11350-11357.	1.5	12
22	Theoretical Investigations on the Possibility of Prebiotic HCN Formation via O-Addition Reactions. Journal of Physical Chemistry A, 2020, 124, 4782-4792.	1.1	8
23	Structural rigidity accelerates quantum decoherence and extends carrier lifetime in porphyrin nanoballs: a time domain atomistic simulation. Nanoscale Advances, 2020, 2, 1502-1511.	2.2	8
24	Comparative Study on the Photovoltaic Properties of ZnX (X = S, Se, Te) QD/CNT Inorganic/Organic Hybrid Nanocomposites. Journal of Physical Chemistry C, 2020, 124, 7652-7660.	1.5	12
25	Triazine- and Keto-Functionalized Porous Covalent Organic Framework as a Promising Anode Material for Na-Ion Batteries: A First-Principles Study. Journal of Physical Chemistry C, 2020, 124, 15870-15878.	1.5	22
26	Silicon and Phosphorus Co-doped Bipyridine-Linked Covalent Triazine Framework as a Promising Metal-Free Catalyst for Hydrogen Evolution Reaction: A Theoretical Investigation. Journal of Physical Chemistry Letters, 2020, 11, 1542-1549.	2.1	37
27	Molecular design of porphyrin dyes using different electron-withdrawing moieties for high performance dye-sensitized solar cells. Computational and Theoretical Chemistry, 2020, 1182, 112846.	1.1	5
28	Edge-Modified Phosphorene Antidot Nanoflakes and Their van der Waals Heterojunctions for Solar Cell Applications. Journal of Physical Chemistry C, 2019, 123, 20748-20756.	1.5	15
29	Periodically-ordered one and two dimensional CdTe QD superstructures: a path forward in photovoltaics. Physical Chemistry Chemical Physics, 2019, 21, 19391-19402.	1.3	10
30	Engineering the magnetic properties of PtSe₂ monolayer through transition metal doping. Journal of Physics Condensed Matter, 2019, 31, 145502.	0.7	36
31	Role of Chalcogens in the Exciton Relaxation Dynamics of Chalcogenol-Functionalized CdSe QD: A Time-Domain Atomistic Simulation. Chemistry of Materials, 2019, 31, 4042-4050.	3.2	20
32	Can Remote N-Heterocyclic Carbenes Be Used for Designing Efficient Blue Triplet Emitters? An Answer from Quantum Chemical Investigation. Journal of Physical Chemistry C, 2019, 123, 14216-14222.	1.5	4
33	Charge transport and transfer phenomena involving conjugated acenes and heteroacenes. Bulletin of Materials Science, 2019, 42, 1.	0.8	3
34	Molecular engineering of anchoring groups for designing efficient triazatruxene-based organic dye-sensitized solar cells. New Journal of Chemistry, 2019, 43, 6480-6491.	1.4	15
35	Unambiguous hydrogenation of CO₂ by coinage-metal hydride anions: an intuitive idea based on in silico experiments. Physical Chemistry Chemical Physics, 2019, 21, 7483-7490.	1.3	13
36	Pathways for Improving the Photovoltaic Efficiency of Porphyrin and Phosphorene Antidot Lattice Nanocomposites: An Insight from a Theoretical Study. Journal of Physical Chemistry C, 2019, 123, 5303-5311.	1.5	18

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37	Computational Investigation on the Electronic Structure and Functionalities of a Thiophene-Based Covalent Triazine Framework. ACS Omega, 2019, 4, 3556-3564.	1.6	12
38	Mechanistic insights into the non-bifunctional hydrogenation of esters by Co(<scp>ii</scp>) pincer complexes: a DFT study. Dalton Transactions, 2019, 48, 16083-16090.	1.6	5
39	Two-Dimensional Covalent Triazine Framework as a Promising Anode Material for Li-Ion Batteries. Journal of Physical Chemistry C, 2019, 123, 30155-30164.	1.5	34
40	CH₃NO as a potential intermediate for early atmospheric HCN: a quantum chemical insight. Physical Chemistry Chemical Physics, 2019, 21, 25126-25138.	1.3	5
41	Bulky, dendronized iridium complexes and their photoluminescence. Journal of Materials Chemistry C, 2019, 7, 15252-15258.	2.7	5
42	Charge transport through nanocontacts. Chemical Modelling, 2019, , 70-130.	0.2	3
43	Engineering the Electronic Structure of Tin Sulfide Nanoribbons: A Computational Study. Journal of Physical Chemistry C, 2018, 122, 5731-5741.	1.5	18
44	Multifunctionalities of an Azine-Linked Covalent Organic Framework: From Nanoelectronics to Nitroexplosive Detection and Conductance Switching. Journal of Physical Chemistry C, 2018, 122, 3245-3255.	1.5	27
45	Fisher information of two-electron systems. European Physical Journal Plus, 2018, 133, 1.	1.2	9
46	Tuning the BODIPY core for its potential use in DSSC: a quantum chemical approach. Bulletin of Materials Science, 2018, 41, 1.	0.8	19
47	Essential Role of Ancillary Ligand in Color Tuning and Quantum Efficiency of Ir(III) Complexes with N-Heterocyclic or Mesoionic Carbene Ligand: A Comparative Quantum Chemical Study. Journal of Physical Chemistry A, 2018, 122, 7532-7539.	1.1	9
48	Harnessing carbazole based small molecules for the synthesis of the fluorescent gold nanoparticles: A unified experimental and theoretical approach to understand the mechanism of synthesis. Colloids and Surfaces B: Biointerfaces, 2018, 172, 440-450.	2.5	5
49	Computational design of some TTF-substituted acene-based dyes for solar cell application using hollow ZnO quantum dot as acceptor. Computational and Theoretical Chemistry, 2018, 1136-1137, 10-17.	1.1	11
50	Porous Grapheneâ€“Fullerene Nanocomposites: A New Composite for Solar Cell and Optoelectronic Applications. Journal of Physical Chemistry C, 2018, 122, 15835-15842.	1.5	22
51	Computational studies on the hydride transfer barrier for the catalytic hydrogenation of CO2 by different Ni(II) complexes. Journal of Molecular Modeling, 2018, 24, 224.	0.8	10
52	Computational Design of Quaterpyridineâ€Based Fe/Mnâ€“Complexes for the Direct Hydrogenation of CO 2 to HCOOH: A Direction for Atomâ€Economic Approach. ChemistrySelect, 2018, 3, 5185-5193.	0.7	6
53	Controlling the charge transfer and recombination dynamics in hollow ZnO QD based dye sensitized solar cell: An insight from ab initio simulation. Chemical Physics Letters, 2018, 709, 21-25.	1.2	10
54	Substitution induced carrier switching in S,N-heteroacene molecular junctions: A first principle analysis. Chemical Physics Letters, 2018, 708, 87-93.	1.2	12

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55	Origin of Different Photovoltaic Activities in Regioisomeric Small Organic Molecule Solar Cells: The Intrinsic Role of Charge Transfer Processes. Journal of Physical Chemistry C, 2018, 122, 14296-14303.	1.5	18
56	Effect of additional donor group on the charge transfer/recombination dynamics of a photoactive organic dye: A quantum mechanical investigation. Computational and Theoretical Chemistry, 2017, 1103, 38-47.	1.1	20
57	A Theoretical Perspective on the Photovoltaic Performance of S,N-Heteroacenes: An Evenâ€“Odd Effect on the Charge Separation Dynamics. Journal of Physical Chemistry C, 2017, 121, 2574-2587.	1.5	56
58	Is the Metallic Phosphorus Carbide (Î²₀-PC) Monolayer Stable? An Answer from a Theoretical Perspective. Journal of Physical Chemistry Letters, 2017, 8, 747-754.	2.1	47
59	Computational studies on the mechanism and selectivity of Al8O12 nanocluster for different elimination reactions. Structural Chemistry, 2017, 28, 1895-1906.	1.0	9
60	Engineering the electronic structure of zigzag graphene nanoribbons with periodic line defect. Physics Letters, Section A: General, Atomic and Solid State Physics, 2017, 381, 307-313.	0.9	16
61	Quantum chemical investigation on the Ir(<scp>iii</scp>) complexes with an isomeric triazine-based imidazolium carbene ligand for efficient blue OLEDs. Physical Chemistry Chemical Physics, 2017, 19, 29629-29640.	1.3	16
62	Phosphorene quantum dot-fullerene nanocomposites for solar energy conversion: An unexplored inorganic-organic nanohybrid with novel photovoltaic properties. Chemical Physics Letters, 2017, 685, 16-22.	1.2	25
63	Bis(dithioline)-Based Metalâ€“Organic Frameworks with Superior Electronic and Magnetic Properties: Spin Frustration to Spintronics and Gas Sensing. Journal of Physical Chemistry C, 2016, 120, 28307-28319.	1.5	55
64	Quantum transport behavior of Ni-based dinuclear complexes in presence of zigzag graphene nanoribbon as electrode. Chemical Physics, 2016, 478, 173-177.	0.9	6
65	Theoretical studies on the photophysical properties of some Iridium (III) complexes used for OLED. Journal of Physics and Chemistry of Solids, 2016, 96-97, 100-106.	1.9	21
66	Computational studies on the reactivity of alkyl halides over (Al₂O₃)_nnanoclusters: an approach towards room temperature dehydrohalogenation. Nanoscale, 2016, 8, 10205-10218.	2.8	21
67	Isoelectronically doped CdSe/Te nanoalloys as alternative solar cell materials: insight from computational analysis. RSC Advances, 2016, 6, 86494-86501.	1.7	4
68	Optimizing the Photovoltaic Properties of CdTe Quantum Dotâ€“Porphyrin Nanocomposites: A Theoretical Study. Journal of Physical Chemistry C, 2016, 120, 17878-17886.	1.5	24
69	Tuning the phosphorescence and quantum efficiency of heteroleptic Ir(III) complexes based on pyridine-tetrazole as an ancillary ligand: An overview from quantum chemical investigations. Computational and Theoretical Chemistry, 2016, 1092, 32-40.	1.1	20
70	Coronene-based metalâ€“organic framework: a theoretical exploration. Physical Chemistry Chemical Physics, 2016, 18, 25277-25283.	1.3	21
71	Understanding the Electronic Structure of Graphene Quantum Dot-Fullerene Nanohybrids for Photovoltaic Applications. Zeitschrift Fur Physikalische Chemie, 2016, 230, 777-790.	1.4	14
72	Superiority of Dâ€“Aâ€“D over Dâ€“A type of organic dyes for the application in dye-sensitized solar cell. Chemical Physics Letters, 2016, 649, 23-28.	1.2	20

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73	Energetic and electronic structure of penta-graphene nanoribbons. Carbon, 2016, 100, 118-125.	5.4	97
74	Exploring the electronic structure of nanohybrid materials for their application in solar cell. Chemical Modelling, 2016, , 27-71.	0.2	0
75	Understanding the conductance switching of permethyloligosilanes: A theoretical approach. Journal of Chemical Physics, 2015, 143, 114314.	1.2	8
76	Pentaceneâ€“fullerene bulk-heterojunction solar cell: A computational study. Physics Letters, Section A: General, Atomic and Solid State Physics, 2015, 379, 1036-1042.	0.9	32
77	Theoretical Studies on Understanding the Feasibility of Porphyrin-Sensitized Graphene Quantum Dot Solar Cell. Journal of Physical Chemistry C, 2015, 119, 3400-3407.	1.5	60
78	A new two-dimensional metalâ€“organic framework with high spin-filtering efficiency. Physical Chemistry Chemical Physics, 2015, 17, 17437-17444.	1.3	22
79	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.	1.2	4
80	Theoretical studies on the carrier tunability of oxidized oligothiophenes. Physical Chemistry Chemical Physics, 2015, 17, 26703-26709.	1.3	9
81	The electronic and optical properties of MoS_{2(1â^'x)}Se_{2x}and MoS_{2(1â^'x)}Te_{2x}monolayers. Physical Chemistry Chemical Physics, 2015, 17, 26166-26174.	1.3	60
82	Platinum atomic wire encapsulated in gold nanotubes: A first principle study. , 2014, , .		0
83	Understanding the electronic structure of CdSe quantum dot-fullerene (C60) hybrid nanostructure for photovoltaic applications. Journal of Applied Physics, 2014, 116, .	1.1	16
84	Multisurface Multimode Molecular Dynamical Simulation of Naphthalene and Anthracene Radical Cations by Using Nearly Linear Scalable Time-Dependent Discrete Variable Representation Method. Journal of Physical Chemistry A, 2014, 118, 11451-11470.	1.1	18
85	Controlling the electronic energy levels of ZnO quantum dots using mixed capping ligands. RSC Advances, 2014, 4, 1640-1645.	1.7	16
86	Electronic structure and bandgap engineering of CdTe nanotubes and designing the CdTe nanotubeâ€“fullerene hybrid nanostructures for photovoltaic applications. RSC Advances, 2014, 4, 14673.	1.7	18
87	Doped defective graphene nanoribbons: a new class of materials with novel spin filtering properties. RSC Advances, 2014, 4, 49946-49952.	1.7	13
88	Modulating triphenylamine-based organic dyes for their potential application in dye-sensitized solar cells: a first principle theoretical study. Physical Chemistry Chemical Physics, 2014, 16, 25280-25287.	1.3	38
89	Understanding the interaction of DNAâ€“RNA nucleobases with different ZnO nanomaterials. Physical Chemistry Chemical Physics, 2014, 16, 15355.	1.3	63
90	Band gap engineering of grapheneâ€“CdTe quantum dot hybrid nanostructures. Journal of Materials Chemistry C, 2014, 2, 8967-8975.	2.7	30

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91	Effect of edge states on the transport properties of pentaceneâ€“graphene nanojunctions. Chemical Physics Letters, 2014, 597, 1-5.	1.2	16
92	Tuning the Energy Levels of ZnO/ZnS Core/Shell Nanowires To Design an efficient Nanowire-Based Dye-Sensitized Solar Cell. Journal of Physical Chemistry C, 2013, 117, 15890-15900.	1.5	51
93	NEARLY LINEAR SCALABILITY OF TIME-DEPENDENT DISCRETE VARIABLE REPRESENTATION (TDDVR) METHOD FOR THE DYNAMICS OF MULTI-SURFACE MULTI-MODE HAMILTONIAN. Journal of Theoretical and Computational Chemistry, 2013, 12, 1350042.	1.8	9
94	Pure carbon-based Schottky diode, an implication of stretched carbon nanowire. Journal of Applied Physics, 2013, 114, .	1.1	6
95	Theoretical prediction of a new two-dimensional carbon allotrope and NDR behaviour of its one-dimensional derivatives. Physical Chemistry Chemical Physics, 2013, 15, 21001.	1.3	63
96	Electronic structure of ZnO/ZnS core/shell quantum dots. Chemical Physics Letters, 2013, 555, 191-195.	1.2	18
97	Ligand mediated tuning of the electronic energy levels of ZnO nanoparticles. RSC Advances, 2013, 3, 532-539.	1.7	14
98	Chair like NiAu6: Clusters assemblies and CO oxidation study by ab initio methods. Chemical Physics Letters, 2013, 584, 108-112.	1.2	13
99	Energetics and Electronic Structure of Encapsulated Graphene Nanoribbons in Carbon Nanotube. Journal of Physical Chemistry A, 2013, 117, 8568-8575.	1.1	15
100	Adsorption of Eu atom at the TiO[sub 2] anatase (101) and rutile (110) surfaces. , 2013, , .		1
101	DFT study of H[sub 2]O adsorption on TiO[sub 2] (110) and SnO[sub 2] (110) surfaces. AIP Conference Proceedings, 2013, , .	0.3	8
102	Transition metal dimer on Au(111) surface: A first principle study. , 2012, , .		0
103	Exploring the electronic structure of graphene quantum dots. Journal of Nanoparticle Research, 2012, 14, 1.	0.8	59
104	Explicit Spectral Response of the Geometrical Isomers of a Bio-Active Pyrazoline Derivative Encapsulated in Î²-Cyclodextrin Nanocavity: A Photophysical and Quantum Chemical Analysis. Journal of Physical Chemistry A, 2012, 116, 10371-10382.	1.1	30
105	Electronic Structure of Thiol-Capped CdTe Quantum Dots and CdTeQDâ€“Carbon Nanotube Nanocomposites. Journal of Physical Chemistry C, 2012, 116, 21601-21608.	1.5	19
106	Influence of Sn interaction on the structural evolution of Au clusters: A first principles study. Chemical Physics Letters, 2012, 543, 121-126.	1.2	9
107	Doped GNR pâ€“n Junction as High Performance NDR and Rectifying Device. Journal of Physical Chemistry C, 2012, 116, 18064-18069.	1.5	78
108	Electronic structure and band gap engineering of CdTe semiconductor nanowires. Journal of Materials Chemistry, 2012, 22, 10716.	6.7	32

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109	Electronic structure and transport properties of sulfur-passivated graphene nanoribbons. Journal of Applied Physics, 2012, 112, .	1.1	13
110	Tuning the HOMOâ€“LUMO gap of SiC quantum dots by surface functionalization. Chemical Physics Letters, 2012, 536, 118-122.	1.2	17
111	A complete set of selfâ€consistent charge densityâ€functional tightâ€binding parametrization of zinc chalcogenides (ZnX; X=O, S, Se, and Te). Journal of Computational Chemistry, 2012, 33, 1165-1178.	1.5	30
112	Self-Consistent-Charge Density-Functional Tight-Binding Parameters for Cdâ€“X (X = S, Se, Te) Compounds and Their Interaction with H, O, C, and N. Journal of Chemical Theory and Computation, 2011, 7, 2262-2276.	2.3	45
113	Size-dependent electronic structure of rutile TiO2 quantum dots. Chemical Physics Letters, 2011, 516, 68-71.	1.2	20
114	Oxidation of tin clusters: A first principles study. Chemical Physics Letters, 2011, 518, 70-75.	1.2	3
115	The Fourier grid Hamiltonian method for calculating vibrational energy levels of triatomic molecules. International Journal of Quantum Chemistry, 2011, 111, 2268-2274.	1.0	5
116	Size and composition dependent electronic and optical properties of GaxAl1â^'xAs and AlxGa1â^'xAs alloyed nanocrystals. Applied Physics Letters, 2009, 94, 123105.	1.5	5
117	A theoretical study on the electronic structure of GaAs/AlAs and AlAs/GaAs core/shell nanoparticles. Journal of Physics and Chemistry of Solids, 2009, 70, 1024-1029.	1.9	2
118	Theoretical prediction of ring structures for ZnS quantum dots. Chemical Physics Letters, 2009, 467, 365-368.	1.2	9
119	Structural, Energetic, and Mechanical Properties of ZnSe Nanotubes. Journal of Physical Chemistry C, 2009, 113, 6439-6443.	1.5	18
120	A search for lowest energy structures of ZnS quantum dots: Genetic algorithm tight-binding study. Journal of Chemical Physics, 2009, 130, 214703.	1.2	18
121	A Theoretical Study on the Electronic Structure of ZnSe/ZnS and ZnS/ZnSe Core/Shell Nanoparticles. Journal of Physical Chemistry C, 2008, 112, 11630-11636.	1.5	40
122	Size-Dependent Properties of Hollow ZnS Nanoclusters. Journal of Physical Chemistry C, 2008, 112, 6307-6312.	1.5	31
123	Theoretical studies of the effect of surface passivation on structural, electronic, and optical properties of zinc selenide clusters. Physical Review B, 2007, 76, .	1.1	26
124	Theoretical Study of the Electronic Structure of GaAs Nanotubes. Journal of Physical Chemistry C, 2007, 111, 12284-12288.	1.5	11
125	Theoretical Study on the Structural, Energetic, and Optical Properties of ZnS Nanotube. Journal of Physical Chemistry C, 2007, 111, 1556-1559.	1.5	26
126	Controlling the Shape of Nanocrystals. Journal of Physical Chemistry C, 2007, 111, 16071-16075.	1.5	7

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127	Theoretical investigation of structural and electronic properties of wurtzite clusters. Journal of Physics and Chemistry of Solids, 2007, 68, 1324-1329.	1.9	1
128	Fourier grid Hamiltonian-based multidimensional Floquet propagator method for continuous, pulsed, and bichromatic laser field: Application to the multiphoton dissociation dynamics of HCN molecule. International Journal of Quantum Chemistry, 2007, 107, 1285-1294.	1.0	10
129	Effects of barrier fluctuation on the tunneling dynamics in the presence of classical chaos in a mixed quantum-classical system. Pramana - Journal of Physics, 2007, 68, 377-387.	0.9	0
130	Theoretical studies of structural and electronic properties of AlnAsn clusters. International Journal of Quantum Chemistry, 2006, 106, 887-893.	1.0	3
131	Theoretical study of structural, electronic, and optical properties ofZnmSenclusters. Physical Review B, 2006, 73, .	1.1	35
132	A theoretical study of the structural and electronic properties of CdSe/CdS and CdS/CdSe core/shell nanoparticles. Chemical Physics Letters, 2005, 405, 103-107.	1.2	34
133	Theoretical studies on size-dependent properties of GanAsn clusters. Chemical Physics Letters, 2005, 407, 498-503.	1.2	14
134	The Effects of Organisation, Embedding and Surfactants on the Properties of Cadmium Chalcogenide (CdS, CdSe and CdS/CdSe) Semiconductor Nanoparticles. European Journal of Inorganic Chemistry, 2005, 2005, 3585-3596.	1.0	33
135	The Effects of Organization, Embedding and Surfactants on the Properties of Cadmium Chalcogenide (CdS, CdSe and CdS/CdSe) Semiconductor Nanoparticles. ChemInform, 2005, 36, no.	0.1	0
136	Effects of thermal modulation on tunneling through a fluctuating barrier in presence of bichromatic electromagnetic field. International Journal of Quantum Chemistry, 2005, 103, 388-393.	1.0	1
137	Size-dependent properties of ZnmSn clusters: A density-functional tight-binding study. Journal of Chemical Physics, 2005, 123, 044311.	1.2	39
138	Tunneling through a fluctuating barrier in the presence of a periodically driving field. International Journal of Quantum Chemistry, 2004, 97, 914-921.	1.0	5
139	Tunneling through a fluctuating barrier in presence of bichromatic electromagnetic field. Physics Letters, Section A: General, Atomic and Solid State Physics, 2004, 323, 389-394.	0.9	3
140	Momentum densities and Compton profiles of alkali-metal atoms. Pramana - Journal of Physics, 2003, 60, 483-490.	0.9	0
141	Tunneling dynamics of a double-well oscillator: Effects of barrier fluctuation and thermal modulation. International Journal of Quantum Chemistry, 2003, 93, 280-285.	1.0	5
142	Structural and electronic properties of thin chains of Ag. Physical Review B, 2003, 68, .	1.1	26
143	Density-functional study of size-dependent properties ofCdmSenclusters. Physical Review B, 2003, 68, .	1.1	63
144	Stability and bandgap of semiconductor clusters. Chemical Physics Letters, 2002, 365, 75-81.	1.2	57

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145	Calculating pure rotational transitions of water molecule with a simple Lanczos method. Pramana - Journal of Physics, 2001, 56, 537-543.	0.9	0
146	Molecular Structure and Packing in the Crystalline State of 4-n-Ethyl-4â€²-Cyanobiphenyl (2CB) by Single Crystal X-ray Diffractometry. Molecular Crystals and Liquid Crystals, 1998, 325, 91-97.	0.3	5
147	Size-dependent electronic structure of semiconductor nanoparticles. Chemical Modelling, 0, , 135-167.	0.2	3