Swapan K Ghosh

List of Publications by Year
in descending order

92	3,345	168829 31	169272 56
papers	citations	h-index	g-index

93	93	93	3518
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Dynamics in condensed phase for systems involving phase functions obeying Gaussian statistics. Journal of the Indian Chemical Society, 2022, 99, 100290.	1.3	0
2	Concept of reaction coordinate for dynamics of optically controlled non-equilibrium processes in condensed phase. Theoretical Chemistry Accounts, 2020, 139, 1.	0.5	1
3	Reactivity Parameters and Substitution Effect in Organic Acids. Journal of Physical Chemistry A, 2020, 124, 3770-3777.	1.1	5
4	Ruthenium(II)â€“arene complexes of diimines: Effect of diimine intercalation and hydrophobicity on DNA and protein binding and cytotoxicity. Applied Organometallic Chemistry, 2018, 32, e4154.	1.7	14
5	Insight into the enhanced photocatalytic activity of SrTiO3 in the presence of a (Ni, V/Nb/Ta/Sb) pair. Physical Chemistry Chemical Physics, 2018, 20, 20078-20087.	1.3	23
6	Improving visible light photocatalytic activity of KTaO3 using cation-anion dopant pair. Solar Energy Materials and Solar Cells, 2017, 159, 590-598.	3.0	31
7	DNA and protein binding, double-strand DNA cleavage and cytotoxicity of mixed ligand copper(II) complexes of the antibacterial drug nalidixic acid. Journal of Inorganic Biochemistry, 2017, 174, 1-13.	1.5	69
8	A computational investigation of the red and blue shifts in hydrogen bonded systems. Journal of Chemical Sciences, 2017, 129, 975-981.	0.7	7
9	Efficient Strategy for Enhancement of Visible Light Photocatalytic Activity of NaTaO₃ by a Significant Extent. Journal of Physical Chemistry C, 2017, 121, 12980-12990.	1.5	20
10	Optically Controlled Electron-Transfer Reaction Kinetics and Solvation Dynamics: Effect of Franckâ€“Condon States. Journal of Physical Chemistry Letters, 2017, 8, 4545-4549.	2.1	7
11	An Efficient Strategy for Controlled Band Gap Engineering of KTaO₃. Journal of Physical Chemistry C, 2016, 120, 6920-6929.	1.5	63
12	Improving the photocatalytic activity of s-triazine based graphitic carbon nitride through metal decoration: an ab initio investigation. Physical Chemistry Chemical Physics, 2016, 18, 26466-26474.	1.3	16
13	Improving visible light photocatalytic activity of NaNbO₃: a DFT based investigation. RSC Advances, 2016, 6, 90188-90196.	1.7	21
14	Improving KNbO₃ photocatalytic activity under visible light. RSC Advances, 2016, 6, 9958-9966.	1.7	33
15	Exploring the Role of La Codoping beyond Charge Compensation for Enhanced Hydrogen Evolution by Rhâ€“SrTiO₃. Journal of Physical Chemistry B, 2015, 119, 11089-11098.	1.2	54
16	Effects of Concentration on Like-Charge Pairing of Guanidinium Ions and on the Structure of Water: An All-Atom Molecular Dynamics Simulation Study. Journal of Physical Chemistry B, 2015, 119, 11262-11274.	1.2	27
17	Origin of enhanced visible light driven water splitting by (Rh, Sb)-SrTiO₃. Physical Chemistry Chemical Physics, 2015, 17, 15274-15283.	1.3	40
18	Hydrogen Trapping Ability of the Pyridineâ€“Lithium⁺ (1:1) Complex. Journal of Physical Chemistry A, 2015, 119, 3056-3063.	1.1	18

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19	Role of F in Improving the Photocatalytic Activity of Rh-Doped SrTiO₃. Journal of Physical Chemistry C, 2015, 119, 7215-7224.	1.5	56
20	Photocatalytic splitting of water on s-triazine based graphitic carbon nitride: an ab initio investigation. Journal of Materials Chemistry A, 2015, 3, 23011-23016.	5.2	53
21	Enhancement of Visible Light Photocatalytic Activity of SrTiO₃: A Hybrid Density Functional Study. Journal of Physical Chemistry C, 2015, 119, 23503-23514.	1.5	78
22	Towards an exact factorization of the molecular wave function. Molecular Physics, 2015, 113, 3067-3072.	0.8	4
23	Effect of confinement on the structure and energetics of Zundel cation present inside the hydrophobic carbon nanotubes: an ab initio study. Theoretical Chemistry Accounts, 2014, 133, 1.	0.5	3
24	Photocatalytic Activity of NaTaO₃ Doped with N, Mo, and (N,Mo): A Hybrid Density Functional Study. Journal of Physical Chemistry C, 2014, 118, 10711-10719.	1.5	59
25	Hydrogen adsorption in lithium decorated conjugated microporous polymers: a DFT investigation. RSC Advances, 2014, 4, 4170-4176.	1.7	19
26	Improving photocatalytic properties of SrTiO₃through (Sb, N) codoping: a hybrid density functional study. RSC Advances, 2014, 4, 45703-45709.	1.7	31
27	Porous Graphitic Carbon Nitride: A Possible Metal-free Photocatalyst for Water Splitting. Journal of Physical Chemistry C, 2014, 118, 26479-26484.	1.5	172
28	Improvement of photocatalytic activity of NaTaO 3 under visible light by N and F doping. Chemical Physics Letters, 2014, 613, 54-58.	1.2	24
29	Zeta potential of colloidal particle in solvent primitive model electrolyte solution: a density functional theory study. Molecular Physics, 2013, 111, 489-496.	0.8	6
30	Density functional theory of surface tension of real fluids using a double well type Helmholtz free energy functional: application to water and heavy water. Molecular Physics, 2013, 111, 589-593.	0.8	3
31	Isomers of C12N12 as potential hydrogen storage materials and the effect of the electric field therein. RSC Advances, 2013, 3, 6991.	1.7	12
32	Density functional theory of vapor to liquid heterogeneous nucleation: Lennardâ€“Jones fluid on solid substrate. Molecular Physics, 2013, 111, 868-877.	0.8	3
33	Comparison of orders, structures and anomalies of water: A molecular dynamics simulation study. , 2013, , .		1
34	Solvent primitive model study of structure of colloidal solution in highly charge asymmetric electrolytes. , 2013, , .		1
35	Chemistry of molecules to physics of materials: A unified view through density window at different length scales. , 2012, , .		0
36	Electron transfer reactions in condensed phase: Effect of reversibility. Physical Review E, 2012, 85, 026105.	0.8	8

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37	Transition Metal Decorated Porphyrin-like Porous Fullerene: Promising Materials for Molecular Hydrogen Adsorption. Journal of Physical Chemistry C, 2012, 116, 25184-25189.	1.5	68
38	Electronic Structure, Optical Properties, and Hydrogen Adsorption Characteristics of Supercubane-Based Three-Dimensional Porous Carbon. Journal of Physical Chemistry C, 2012, 116, 25015-25021.	1.5	20
39	On the interaction of uranyl with functionalized fullerenes: a DFT investigation. RSC Advances, 2012, 2, 2994.	1.7	19
40	Theoretical investigation of hydrogen adsorption in all-metal aromatic clusters. RSC Advances, 2012, 2, 2914.	1.7	44
41	Water dissociation on a gold cluster: the effect of carbon nanostructures as a substrate. RSC Advances, 2012, 2, 10262.	1.7	12
42	Hydrogenâ€bonded complexes of nicotine with simple alcohols. International Journal of Quantum Chemistry, 2012, 112, 2787-2793.	1.0	8
43	Graphyne and Graphdiyne: Promising Materials for Nanoelectronics and Energy Storage Applications. Journal of Physical Chemistry C, 2012, 116, 5951-5956.	1.5	430
44	Elucidating the mechanism of binding of chromate to cucurbit[6]uril: a DFT study. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2012, 72, 437-441.	1.6	10
45	Computational investigation of hydrogen adsorption in silicon-lithium binary clusters#. Journal of Chemical Sciences, 2012, 124, 255-260.	0.7	10
46	Water molecule encapsulated in carbon nanotube model systems: effect of confinement and curvature. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	9
47	Elucidating the structures and binding of halide ions bound to cucurbit[6]uril, hemi-cucurbit[6]uril and bambus[6]uril using DFT calculations. RSC Advances, 2011, 1, 1333.	1.7	27
48	Effect of ionic size on the structure of spherical double layers: a Monte Carlo simulation and density functional theory study. Molecular Physics, 2011, 109, 639-644.	0.8	13
49	An ab Initio Investigation of Hydrogen Adsorption in Li-Dopedcloso-Boranes. Journal of Physical Chemistry C, 2011, 115, 1450-1456.	1.5	40
50	Beyond the Goldâ€“Hydrogen Analogy: Doping Gold Cluster with H-atomâ€“O₂ Activation and Reduction of the Reaction Barrier for CO Oxidation. Journal of Physical Chemistry Letters, 2011, 2, 1476-1480.	2.1	42
51	Tuning the Metal Binding Energy and Hydrogen Storage in Alkali Metal Decorated MOF-5 Through Boron Doping: A Theoretical Investigation. Journal of Physical Chemistry C, 2011, 115, 16984-16991.	1.5	45
52	Mapping the reaction dynamics in Liouville space onto a reaction coordinate space: A first-principle-based theory. Physical Review E, 2011, 83, 026104.	0.8	8
53	Theory of reversible electron transfer reactions in a condensed phase. Physical Review E, 2010, 82, 016110.	0.8	13
54	Work distribution for a particle moving in an optical trap and non-Markovian bath. Journal of Chemical Sciences, 2009, 121, 897-904.	0.7	1

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55	A self-consistent density-functional approach to the structure of electric double layer: charge-asymmetric electrolytes. Molecular Physics, 2009, 107, 19-25.	0.8	5
56	One-Dimensional Description of Multidimensional Electron Transfer Reactions in Condensed Phase. Journal of Physical Chemistry A, 2008, 112, 4879-4884.	1.1	4
57	Hydrogen Bonding in Substituted Formic Acid Dimers. Journal of Physical Chemistry A, 2006, 110, 12623-12628.	1.1	48
58	THEORETICAL STUDIES ON POLARIZABILITY OF ALKALI METAL CLUSTERS. , 2006, , 625-655.		0
59	A density functional theory-based chemical potential equalisation approach to molecular polarizability. Journal of Chemical Sciences, 2005, 117, 401-409.	0.7	9
60	Ab initio studies on the polarizability of lithium clusters: Some unusual results. International Journal of Quantum Chemistry, 2005, 105, 166-173.	1.0	21
61	Electron Density and Energy Decomposition Analysis in Hydrogen-Bonded Complexes of Azabenzenes with Water, Acetamide, and Thioacetamide. Journal of Physical Chemistry A, 2005, 109, 7575-7582.	1.1	44
62	Diffusion-Influenced Fluorescence Quenching by Electron Transfer: The Effect of an External Electric Field. Israel Journal of Chemistry, 2004, 44, 119-125.	1.0	1
63	Density functional theory and multiscale materials modeling. Bulletin of Materials Science, 2003, 26, 3-12.	0.8	5
64	Integral equation theory of penetrable sphere fluids: A modified Verlet bridge function approach. Journal of Chemical Physics, 2003, 119, 4827-4832.	1.2	24
65	Diffusion assisted endâ€“toâ€“end relaxation of a flexible Rouse polymer chain: Fluorescence quenching through a model energy transfer. Journal of Chemical Physics, 2003, 119, 572-584.	1.2	13
66	Polarizability of water clusters: Anab initioinvestigation. Journal of Chemical Physics, 2003, 118, 8547-8550.	1.2	42
67	Weighted-density-functional approach to the structure of nonuniform fluids. Journal of Chemical Physics, 2003, 118, 8326-8330.	1.2	6
68	Structure of nonuniform three-component fluid mixtures: A density-functional approach. Journal of Chemical Physics, 2003, 118, 3668-3676.	1.2	21
69	Structure of an inhomogeneous fluid mixture: A new weighted density-functional theory within a perturbative approach. Journal of Chemical Physics, 2003, 118, 1327-1332.	1.2	5
70	Diffusion influenced end-to-end reaction of a flexible polymer chain: The memory effect. Journal of Chemical Physics, 2002, 116, 4366-4369.	1.2	17
71	Structure of electric double layers: A self-consistent weighted-density-functional approach. Journal of Chemical Physics, 2002, 117, 8938-8943.	1.2	45
72	Sedimentation equilibrium of a suspension of adhesive colloidal particles in a planar slit: A density functional approach. Journal of Chemical Physics, 2002, 116, 384.	1.2	11

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73	A self-consistent weighted-density-functional approach to the structure of simple fluids. Journal of Chemical Physics, 2002, 116, 9845-9849.	1.2	6
74	Structure of nonuniform fluid mixtures: A self-consistent density-functional approach. Journal of Chemical Physics, 2002, 117, 8933-8937.	1.2	19
75	A continued fraction approach to cross diffusivity in a binary fluid mixture. Journal of Chemical Physics, 2002, 116, 7081-7086.	1.2	1
76	Integral equation theory of Lennard-Jones fluids: A modified Verlet bridge function approach. Journal of Chemical Physics, 2002, 116, 8517.	1.2	59
77	DENSITY CONCEPT IN MATERIALS MODELING AT DIFFERENT LENGTH SCALES. , 2002, , 1295-1326.		0
78	Universal Scaling Laws of Diffusion in a Binary Fluid Mixture. Physical Review Letters, 2001, 87, 245901.	2.9	93
79	Density functional theory of inhomogeneous fluid mixture based on bridge function. Journal of Chemical Physics, 2001, 114, 8530-8538.	1.2	32
80	Mode coupling theory of self and cross diffusivity in a binary fluid mixture: Application to Lennard-Jones systems. Journal of Chemical Physics, 2001, 114, 10419-10429.	1.2	48
81	Colloidal suspensions in charged cylindrical pores: A perturbative density functional approach. Journal of Chemical Physics, 1999, 111, 1737-1745.	1.2	7
82	Predictive methods of pople. Resonance, 1999, 4, 95-98.	0.2	0
83	A perturbative density functional theory of inhomogeneous fluid mixture. Journal of Chemical Physics, 1999, 110, 8628-8635.	1.2	26
84	A perturbative density functional approach to the structure of colloidal suspension. Journal of Chemical Physics, 1998, 108, 7493-7500.	1.2	12
85	Exchange?correlation potential and excited-state density functional theory. International Journal of Quantum Chemistry, 1996, 60, 535-543.	1.0	17
86	Exact evaluation of diffusion dynamics in a potential well with a general delocalized sink. Physical Review E, 1993, 47, 4568-4571.	0.8	28
87	Density-functional theory of many-electron systems subjected to time-dependent electric and magnetic fields. Physical Review A, 1988, 38, 1149-1158.	1.0	177
88	Toward a semiempirical density functional theory of chemical binding. Theoretica Chimica Acta, 1987, 72, 379-391.	0.9	37
89	A classical fluidâ€like approach to the densityâ€functional formalism of manyâ€electron systems. Journal of Chemical Physics, 1985, 83, 2976-2983.	1.2	191
90	Study of the kinetic energy density functional in the locally linear potential approximation. Journal of Chemical Physics, 1985, 83, 5778-5783.	1.2	48

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91	Chemical Physics, 1985, 82, 3307-3315.	1.2	115
92	On the concept of local hardness in chemistry. Journal of the American Chemical Society, 1985, 107, 6811-6814.	6.6	307