Swapan K Ghosh

List of Publications by Year
in descending order

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92 papers	3,345 citations	147801 31 h-index	149698 56 g-index
93 all docs	93 docs citations	93 times ranked	3083 citing authors

#	Article	IF	Citations
1	Graphyne and Graphdiyne: Promising Materials for Nanoelectronics and Energy Storage Applications. Journal of Physical Chemistry C, 2012, 116, 5951-5956.	3.1	430
2	On the concept of local hardness in chemistry. Journal of the American Chemical Society, 1985, 107, 6811-6814.	13.7	307
3	A classical fluidâ€like approach to the densityâ€functional formalism of manyâ€electron systems. Journal of Chemical Physics, 1985, 83, 2976-2983.	3.0	191
4	Density-functional theory of many-electron systems subjected to time-dependent electric and magnetic fields. Physical Review A, 1988, 38, 1149-1158.	2.5	177
5	Porous Graphitic Carbon Nitride: A Possible Metal-free Photocatalyst for Water Splitting. Journal of Physical Chemistry C, 2014, 118, 26479-26484.	3.1	172
6	Chemical Physics, 1985, 82, 3307-3315.	3.0	115
7	Universal Scaling Laws of Diffusion in a Binary Fluid Mixture. Physical Review Letters, 2001, 87, 245901.	7.8	93
8	Enhancement of Visible Light Photocatalytic Activity of SrTiO₃: A Hybrid Density Functional Study. Journal of Physical Chemistry C, 2015, 119, 23503-23514.	3.1	78
9	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.	3.5	69
10	Transition Metal Decorated Porphyrin-like Porous Fullerene: Promising Materials for Molecular Hydrogen Adsorption. Journal of Physical Chemistry C, 2012, 116, 25184-25189.	3.1	68
11	An Efficient Strategy for Controlled Band Gap Engineering of KTaO₃. Journal of Physical Chemistry C, 2016, 120, 6920-6929.	3.1	63
12	Integral equation theory of Lennard-Jones fluids: A modified Verlet bridge function approach. Journal of Chemical Physics, 2002, 116, 8517.	3.0	59
13	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.	3.1	59
14	Role of F in Improving the Photocatalytic Activity of Rh-Doped SrTiO₃. Journal of Physical Chemistry C, 2015, 119, 7215-7224.	3.1	56
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.	2.6	54
16	Photocatalytic splitting of water on s-triazine based graphitic carbon nitride: an ab initio investigation. Journal of Materials Chemistry A, 2015, 3, 23011-23016.	10.3	53
17	Study of the kinetic energy density functional in the locally linear potential approximation. Journal of Chemical Physics, 1985, 83, 5778-5783.	3.0	48
18	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.	3.0	48

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19	Hydrogen Bonding in Substituted Formic Acid Dimers. Journal of Physical Chemistry A, 2006, 110, 12623-12628.	2.5	48
20	Structure of electric double layers: A self-consistent weighted-density-functional approach. Journal of Chemical Physics, 2002, 117, 8938-8943.	3.0	45
21	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.	3.1	45
22	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.	2.5	44
23	Theoretical investigation of hydrogen adsorption in all-metal aromatic clusters. RSC Advances, 2012, 2, 2914.	3.6	44
24	Polarizability of water clusters: Anab initioinvestigation. Journal of Chemical Physics, 2003, 118, 8547-8550.	3.0	42
25	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.	4.6	42
26	An ab Initio Investigation of Hydrogen Adsorption in Li-Dopedcloso-Boranes. Journal of Physical Chemistry C, 2011, 115, 1450-1456.	3.1	40
27	Origin of enhanced visible light driven water splitting by (Rh, Sb)-SrTiO₃. Physical Chemistry Chemical Physics, 2015, 17, 15274-15283.	2.8	40
28	Toward a semiempirical density functional theory of chemical binding. Theoretica Chimica Acta, 1987, 72, 379-391.	0.8	37
29	Improving KNbO₃ photocatalytic activity under visible light. RSC Advances, 2016, 6, 9958-9966.	3.6	33
30	Density functional theory of inhomogeneous fluid mixture based on bridge function. Journal of Chemical Physics, 2001, 114, 8530-8538.	3.0	32
31	Improving photocatalytic properties of SrTiO₃through (Sb, N) codoping: a hybrid density functional study. RSC Advances, 2014, 4, 45703-45709.	3.6	31
32	Improving visible light photocatalytic activity of KTaO3 using cation-anion dopant pair. Solar Energy Materials and Solar Cells, 2017, 159, 590-598.	6.2	31
33	Exact evaluation of diffusion dynamics in a potential well with a general delocalized sink. Physical Review E, 1993, 47, 4568-4571.	2.1	28
34	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.	3.6	27
35	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.	2.6	27
36	A perturbative density functional theory of inhomogeneous fluid mixture. Journal of Chemical Physics, 1999, 110, 8628-8635.	3.0	26

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37	Integral equation theory of penetrable sphere fluids: A modified Verlet bridge function approach. Journal of Chemical Physics, 2003, 119, 4827-4832.	3.0	24
38	Improvement of photocatalytic activity of NaTaO 3 under visible light by N and F doping. Chemical Physics Letters, 2014, 613, 54-58.	2.6	24
39	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.	2.8	23
40	Structure of nonuniform three-component fluid mixtures: A density-functional approach. Journal of Chemical Physics, 2003, 118, 3668-3676.	3.0	21
41	Ab initio studies on the polarizability of lithium clusters: Some unusual results. International Journal of Quantum Chemistry, 2005, 105, 166-173.	2.0	21
42	Improving visible light photocatalytic activity of NaNbO₃: a DFT based investigation. RSC Advances, 2016, 6, 90188-90196.	3.6	21
43	Electronic Structure, Optical Properties, and Hydrogen Adsorption Characteristics of Supercubane-Based Three-Dimensional Porous Carbon. Journal of Physical Chemistry C, 2012, 116, 25015-25021.	3.1	20
44	Efficient Strategy for Enhancement of Visible Light Photocatalytic Activity of NaTaO₃ by a Significant Extent. Journal of Physical Chemistry C, 2017, 121, 12980-12990.	3.1	20
45	Structure of nonuniform fluid mixtures: A self-consistent density-functional approach. Journal of Chemical Physics, 2002, 117, 8933-8937.	3.0	19
46	On the interaction of uranyl with functionalized fullerenes: a DFT investigation. RSC Advances, 2012, 2, 2994.	3.6	19
47	Hydrogen adsorption in lithium decorated conjugated microporous polymers: a DFT investigation. RSC Advances, 2014, 4, 4170-4176.	3.6	19
48	Hydrogen Trapping Ability of the Pyridineâ€“Lithium⁺ (1:1) Complex. Journal of Physical Chemistry A, 2015, 119, 3056-3063.	2.5	18
49	Exchange?correlation potential and excited-state density functional theory. International Journal of Quantum Chemistry, 1996, 60, 535-543.	2.0	17
50	Diffusion influenced end-to-end reaction of a flexible polymer chain: The memory effect. Journal of Chemical Physics, 2002, 116, 4366-4369.	3.0	17
51	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.	2.8	16
52	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.	3.5	14
53	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.	3.0	13
54	Theory of reversible electron transfer reactions in a condensed phase. Physical Review E, 2010, 82, 016110.	2.1	13

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55	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.	1.7	13
56	A perturbative density functional approach to the structure of colloidal suspension. Journal of Chemical Physics, 1998, 108, 7493-7500.	3.0	12
57	Water dissociation on a gold cluster: the effect of carbon nanostructures as a substrate. RSC Advances, 2012, 2, 10262.	3.6	12
58	Isomers of C12N12 as potential hydrogen storage materials and the effect of the electric field therein. RSC Advances, 2013, 3, 6991.	3.6	12
59	Sedimentation equilibrium of a suspension of adhesive colloidal particles in a planar slit: A density functional approach. Journal of Chemical Physics, 2002, 116, 384.	3.0	11
60	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
61	Computational investigation of hydrogen adsorption in silicon-lithium binary clusters#. Journal of Chemical Sciences, 2012, 124, 255-260.	1.5	10
62	A density functional theory-based chemical potential equalisation approach to molecular polarizability. Journal of Chemical Sciences, 2005, 117, 401-409.	1.5	9
63	Water molecule encapsulated in carbon nanotube model systems: effect of confinement and curvature. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	9
64	Mapping the reaction dynamics in Liouville space onto a reaction coordinate space: A first-principle-based theory. Physical Review E, 2011, 83, 026104.	2.1	8
65	Electron transfer reactions in condensed phase: Effect of reversibility. Physical Review E, 2012, 85, 026105.	2.1	8
66	Hydrogenâ€bonded complexes of nicotine with simple alcohols. International Journal of Quantum Chemistry, 2012, 112, 2787-2793.	2.0	8
67	Colloidal suspensions in charged cylindrical pores: A perturbative density functional approach. Journal of Chemical Physics, 1999, 111, 1737-1745.	3.0	7
68	A computational investigation of the red and blue shifts in hydrogen bonded systems. Journal of Chemical Sciences, 2017, 129, 975-981.	1.5	7
69	Optically Controlled Electron-Transfer Reaction Kinetics and Solvation Dynamics: Effect of Franckâ€“Condon States. Journal of Physical Chemistry Letters, 2017, 8, 4545-4549.	4.6	7
70	A self-consistent weighted-density-functional approach to the structure of simple fluids. Journal of Chemical Physics, 2002, 116, 9845-9849.	3.0	6
71	Weighted-density-functional approach to the structure of nonuniform fluids. Journal of Chemical Physics, 2003, 118, 8326-8330.	3.0	6
72	Zeta potential of colloidal particle in solvent primitive model electrolyte solution: a density functional theory study. Molecular Physics, 2013, 111, 489-496.	1.7	6

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73	Density functional theory and multiscale materials modeling. Bulletin of Materials Science, 2003, 26, 3-12.	1.7	5
74	Structure of an inhomogeneous fluid mixture: A new weighted density-functional theory within a perturbative approach. Journal of Chemical Physics, 2003, 118, 1327-1332.	3.0	5
75	A self-consistent density-functional approach to the structure of electric double layer: charge-asymmetric electrolytes. Molecular Physics, 2009, 107, 19-25.	1.7	5
76	Reactivity Parameters and Substitution Effect in Organic Acids. Journal of Physical Chemistry A, 2020, 124, 3770-3777.	2.5	5
77	One-Dimensional Description of Multidimensional Electron Transfer Reactions in Condensed Phase. Journal of Physical Chemistry A, 2008, 112, 4879-4884.	2.5	4
78	Towards an exact factorization of the molecular wave function. Molecular Physics, 2015, 113, 3067-3072.	1.7	4
79	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.	1.7	3
80	Density functional theory of vapor to liquid heterogeneous nucleation: Lennardâ€“Jones fluid on solid substrate. Molecular Physics, 2013, 111, 868-877.	1.7	3
81	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.	1.4	3
82	A continued fraction approach to cross diffusivity in a binary fluid mixture. Journal of Chemical Physics, 2002, 116, 7081-7086.	3.0	1
83	Diffusion-Influenced Fluorescence Quenching by Electron Transfer: The Effect of an External Electric Field. Israel Journal of Chemistry, 2004, 44, 119-125.	2.3	1
84	Work distribution for a particle moving in an optical trap and non-Markovian bath. Journal of Chemical Sciences, 2009, 121, 897-904.	1.5	1
85	Comparison of orders, structures and anomalies of water: A molecular dynamics simulation study. , 2013, , .		1
86	Solvent primitive model study of structure of colloidal solution in highly charge asymmetric electrolytes. , 2013, , .		1
87	Concept of reaction coordinate for dynamics of optically controlled non-equilibrium processes in condensed phase. Theoretical Chemistry Accounts, 2020, 139, 1.	1.4	1
88	Predictive methods of pople. Resonance, 1999, 4, 95-98.	0.3	0
89	THEORETICAL STUDIES ON POLARIZABILITY OF ALKALI METAL CLUSTERS. , 2006, , 625-655.		0
90	Chemistry of molecules to physics of materials: A unified view through density window at different length scales. , 2012, , .		0

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91	DENSITY CONCEPT IN MATERIALS MODELING AT DIFFERENT LENGTH SCALES. , 2002, , 1295-1326.		0
92	Dynamics in condensed phase for systems involving phase functions obeying Gaussian statistics. Journal of the Indian Chemical Society, 2022, 99, 100290.	2.8	0