Prasanjit Samal

List of Publications by Year
in descending order

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48	701	567281 15	642732 23
papers	citations	h-index	g-index

49	49	49	318
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Assessing the performance of the Tao-Mo semilocal density functional in the projector-augmented-wave method. Journal of Chemical Physics, 2018, 149, 044120.	3.0	50
2	Relevance of the Pauli kinetic energy density for semilocal functionals. Physical Review B, 2019, 100, .	3.2	38
3	Assessing the performance of the recent meta-GGA density functionals for describing the lattice constants, bulk moduli, and cohesive energies of alkali, alkaline-earth, and transition metals. Journal of Chemical Physics, 2018, 149, 164703.	3.0	35
4	Efficient band gap prediction of semiconductors and insulators from a semilocal exchange-correlation functional. Physical Review B, 2019, 100, .	3.2	35
5	Improving the Performance of Taoâ€“Mo Non-empirical Density Functional with Broader Applicability in Quantum Chemistry and Materials Science. Journal of Physical Chemistry A, 2019, 123, 6356-6369.	2.5	29
6	Bandgap of two-dimensional materials: Thorough assessment of modern exchangeâ€“correlation functionals. Journal of Chemical Physics, 2021, 155, 104103.	3.0	26
7	Exploring foundations of time-independent density functional theory for excited states. Journal of Physics B: Atomic, Molecular and Optical Physics, 2006, 39, 4065-4080.	1.5	24
8	Screened range-separated hybrid by balancing the compact and slowly varying density regimes: Satisfaction of local density linear response. Journal of Chemical Physics, 2020, 152, 044111.	3.0	22
9	A meta-GGA level screened range-separated hybrid functional by employing short range Hartreeâ€“Fock with a long range semilocal functional. Physical Chemistry Chemical Physics, 2018, 20, 8999-9005.	2.8	21
10	Long-range corrected density functional through the density matrix expansion based semilocal exchange hole. Physical Chemistry Chemical Physics, 2018, 20, 8991-8998.	2.8	21
11	Laplacian free and asymptotic corrected semilocal exchange potential applied to the band gap of solids. Physical Chemistry Chemical Physics, 2019, 21, 19639-19650.	2.8	21
12	Density-to-potential map in time-independent excited-state density-functional theory. Chemical Physics Letters, 2006, 419, 217-222.	2.6	20
13	Improved solid stability from a screened range-separated hybrid functional by satisfying semiclassical atom theory and local density linear response. Physical Review B, 2020, 102, .	3.2	19
14	Efficient Band Structure Calculation of Two-Dimensional Materials from Semilocal Density Functionals. Journal of Physical Chemistry C, 2021, 125, 11206-11215.	3.1	19
15	Local-density approximation for the exchange energy functional in excited-state density functional theory. Journal of Physics B: Atomic, Molecular and Optical Physics, 2005, 38, 3765-3777.	1.5	18
16	Electronic band structure of layers within meta generalized gradient approximation of density functionals. Physical Review B, 2020, 102, .	3.2	18
17	On the many-electron self-interaction error of the semilocal exchange hole based meta-GGA level range-separated hybrid with the B88 hybrids. Chemical Physics Letters, 2018, 713, 1-9.	2.6	17
18	Screened hybrid meta-GGA exchangeâ€“correlation functionals for extended systems. Physical Chemistry Chemical Physics, 2019, 21, 3002-3015.	2.8	16

#	Article	IF	Citations
19	Long-range screened hybrid-functional theory satisfying the local-density linear response. Physical Review A, 2019, 99, .	2.5	16
20	Accurate Water Properties from an Efficient ab Initio Method. Journal of Chemical Theory and Computation, 2020, 16, 974-987.	5.3	15
21	Accurate density functional made more versatile. Journal of Chemical Physics, 2021, 155, 024103.	3.0	15
22	A way of resolving the order-of-limit problem of Taoâ€“Mo semilocal functional. Journal of Chemical Physics, 2020, 153, 184112.	3.0	15
23	Efficient lattice constants and energy bandgaps for condensed systems from a meta-GGA level screened range-separated hybrid functional. Journal of Chemical Physics, 2018, 149, 094105.	3.0	14
24	Performance of Taoâ€“Mo Semilocal Functional with rVV10 Dispersion-Correction: Influence of Different Correlation. Journal of Physical Chemistry A, 2019, 123, 10582-10593.	2.5	14
25	Improved transition metal surface energies from a generalized gradient approximation developed for quasi two-dimensional systems. Journal of Chemical Physics, 2020, 152, 151101.	3.0	14
26	Correct Structural Phase Stability of FeS₂, TiO₂, and MnO₂ from a Semilocal Density Functional. Journal of Physical Chemistry C, 2021, 125, 4284-4291.	3.1	14
27	Insights from the density functional performance of water and waterâ€“solid interactions: SCAN in relation to other meta-GGAs. Journal of Chemical Physics, 2020, 153, 214116.	3.0	14
28	Improving the applicability of the Pauli kinetic energy density based semilocal functional for solids. New Journal of Physics, 2021, 23, 063007.	2.9	13
29	Analysis of Floquet formulation of time-dependent density-functional theory. Chemical Physics Letters, 2006, 433, 204-210.	2.6	12
30	Generalizing Double-Hybrid Density Functionals: Impact of Higher-Order Perturbation Terms. Journal of Chemical Theory and Computation, 2020, 16, 7413-7430.	5.3	12
31	Semilocal Exchange Energy Functional for Two-Dimensional Quantum Systems: A Step Beyond Generalized Gradient Approximations. Journal of Physical Chemistry A, 2017, 121, 4804-4811.	2.5	11
32	Efficient yet accurate dispersion-corrected semilocal exchangeâ€“correlation functionals for non-covalent interactions. Journal of Chemical Physics, 2020, 153, 084117.	3.0	10
33	Gradient approximated exchange energy functionals with improved performances for two-dimensional quantum dot systems. Physica E: Low-Dimensional Systems and Nanostructures, 2018, 97, 268-276.	2.7	9
34	Band Alignment at Heterointerface with Rapid Charge Transfer Supporting Excellent Photocatalytic Degradation of Methylene Blue under Sunlight. Advanced Materials Interfaces, 2022, 9, .	3.7	9
35	A local-density approximation for the exchange energy functional for excited states: The band-gap problem. Physica B: Condensed Matter, 2009, 404, 1137-1142.	2.7	6
36	Time-Independent Excited-State Density Functional Theory. , 2009, , .		5

#	Article	IF	Citations
37	A Parameter-Free Semilocal Exchange Energy Functional for Two-Dimensional Quantum Systems. Journal of Physical Chemistry A, 2018, 122, 3455-3461.	2.5	5
38	Inhomogeneity induced and appropriately parameterized semilocal exchange and correlation energy functionals in two-dimensions. Journal of Chemical Physics, 2018, 148, 134117.	3.0	5
39	Semianalytical wavefunctions and Kohnâ€“Sham exchange-correlation potentials for two-electron atomic systems in two-dimensions. Journal of Physics B: Atomic, Molecular and Optical Physics, 2020, 53, 035001.	1.5	5
40	Benchmark test of a dispersion corrected revised Taoâ€“Mo semilocal functional for thermochemistry, kinetics, and noncovalent interactions of molecules and solids. Journal of Chemical Physics, 2021, 155, 114102.	3.0	4
41	Phase evolution in thermally annealed Ni/Bi multilayers studied by X-ray absorption spectroscopy. Physical Chemistry Chemical Physics, 2022, 24, 4415-4424.	2.8	4
42	Solid-state performance of a meta-GGA screened hybrid density functional constructed from Pauli kinetic enhancement factor dependent semilocal exchange hole. Journal of Chemical Physics, 0, , .	3.0	4
43	Improved electronic structure prediction of chalcopyrite semiconductors from a semilocal density functional based on Pauli kinetic energy enhancement factor. Journal of Physics Condensed Matter, 2022, 34, 075501.	1.8	3
44	Colle-Salvetti type correlation functionals for two-dimensional quantum dot systems. Chemical Physics Letters, 2019, 720, 70-75.	2.6	2
45	Adiabatic connection in density functional theory in two-dimensions: A semi-analytic wavefunction based study for two-electron atomic systems. Journal of Chemical Physics, 2019, 151, 204104.	3.0	1
46	Accurate band gaps from exchange potentials designed from cuspless hydrogen density-based exchange hole model. Physical Chemistry Chemical Physics, 0, , .	2.8	1
47	Exploration of near the origin and the asymptotic behaviors of the Kohn-Sham kinetic energy density for two-dimensional quantum dot systems with parabolic confinement. Journal of Chemical Physics, 2018, 148, 024111.	3.0	0
48	Renormalization group analysis of weakly interacting van der Waals Fermi system. Journal of Physics Condensed Matter, 2021, 33, 335604.	1.8	0