Subrata Jana

List of Publications by Year in descending order

36 papers	585 citations	623734 14 h-index	677142 22 g-index
37 all docs	37 docs citations	37 times ranked	262 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 Tao–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 exchange–correlation functionals. Journal of Chemical Physics, 2021, 155, 104103.	3.0	26
7	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
8	A meta-GGA level screened range-separated hybrid functional by employing short range Hartree–Fock with a long range semilocal functional. Physical Chemistry Chemical Physics, 2018, 20, 8999-9005.	2.8	21
9	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
10	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
11	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
12	Efficient Band Structure Calculation of Two-Dimensional Materials from Semilocal Density Functionals. Journal of Physical Chemistry C, 2021, 125, 11206-11215.	3.1	19
13	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
14	Screened hybrid meta-GGA exchange–correlation functionals for extended systems. Physical Chemistry Chemical Physics, 2019, 21, 3002-3015.	2.8	16
15	Long-range screened hybrid-functional theory satisfying the local-density linear response. Physical Review A, 2019, 99, .	2.5	16
16	Accurate Water Properties from an Efficient ab Initio Method. Journal of Chemical Theory and Computation, 2020, 16, 974-987.	5.3	15
17	Accurate density functional made more versatile. Journal of Chemical Physics, 2021, 155, 024103.	3.0	15
18	A way of resolving the order-of-limit problem of Tao–Mo semilocal functional. Journal of Chemical Physics, 2020, 153, 184112.	3.0	15

#	Article	IF	Citations
19	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
20	Performance of Tao–Mo Semilocal Functional with rVV10 Dispersion-Correction: Influence of Different Correlation. Journal of Physical Chemistry A, 2019, 123, 10582-10593.	2.5	14
21	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
22	Correct Structural Phase Stability of FeS_2, TiO_2, and MnO_2 from a Semilocal Density Functional. Journal of Physical Chemistry C, 2021, 125, 4284-4291.	3.1	14
23	Insights from the density functional performance of water and water–solid interactions: SCAN in relation to other meta-GGAs. Journal of Chemical Physics, 2020, 153, 214116.	3.0	14
24	Improving the applicability of the Pauli kinetic energy density based semilocal functional for solids. New Journal of Physics, 2021, 23, 063007.	2.9	13
25	Generalizing Double-Hybrid Density Functionals: Impact of Higher-Order Perturbation Terms. Journal of Chemical Theory and Computation, 2020, 16, 7413-7430.	5.3	12
26	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
27	Efficient yet accurate dispersion-corrected semilocal exchange–correlation functionals for non-covalent interactions. Journal of Chemical Physics, 2020, 153, 084117.	3.0	10
28	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
29	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
30	A Parameter-Free Semilocal Exchange Energy Functional for Two-Dimensional Quantum Systems. Journal of Physical Chemistry A, 2018, 122, 3455-3461.	2.5	5
31	Inhomogeneity induced and appropriately parameterized semilocal exchange and correlation energy functionals in two-dimensions. Journal of Chemical Physics, 2018, 148, 134117.	3.0	5
32	Benchmark test of a dispersion corrected revised Tao–Mo semilocal functional for thermochemistry, kinetics, and noncovalent interactions of molecules and solids. Journal of Chemical Physics, 2021, 155, 114102.	3.0	4
33	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
34	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
35	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
36	Renormalization group analysis of weakly interacting van der Waals Fermi system. Journal of Physics Condensed Matter, 2021, 33, 335604.	1.8	0