

Subrata Jana

List of Publications by Year in descending order

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#	ARTICLE	IF	CITATIONS
1	Improved electronic structure prediction of chalcopyrite semiconductors from a semilocal density functional based on Pauli kinetic energy enhancement factor. <i>Journal of Physics Condensed Matter</i> , 2022, 34, 075501.	1.8	3
2	Band Alignment at Heterointerface with Rapid Charge Transfer Supporting Excellent Photocatalytic Degradation of Methylene Blue under Sunlight. <i>Advanced Materials Interfaces</i> , 2022, 9, .	3.7	9
3	Correct Structural Phase Stability of FeS ₂ , TiO ₂ , and MnO ₂ from a Semilocal Density Functional. <i>Journal of Physical Chemistry C</i> , 2021, 125, 4284-4291.	3.1	14
4	Efficient Band Structure Calculation of Two-Dimensional Materials from Semilocal Density Functionals. <i>Journal of Physical Chemistry C</i> , 2021, 125, 11206-11215.	3.1	19
5	Improving the applicability of the Pauli kinetic energy density based semilocal functional for solids. <i>New Journal of Physics</i> , 2021, 23, 063007.	2.9	13
6	Renormalization group analysis of weakly interacting van der Waals Fermi system. <i>Journal of Physics Condensed Matter</i> , 2021, 33, 335604.	1.8	0
7	Accurate density functional made more versatile. <i>Journal of Chemical Physics</i> , 2021, 155, 024103.	3.0	15
8	Benchmark test of a dispersion corrected revised Tao-Mo semilocal functional for thermochemistry, kinetics, and noncovalent interactions of molecules and solids. <i>Journal of Chemical Physics</i> , 2021, 155, 114102.	3.0	4
9	Bandgap of two-dimensional materials: Thorough assessment of modern exchange-correlation functionals. <i>Journal of Chemical Physics</i> , 2021, 155, 104103.	3.0	26
10	Accurate Water Properties from an Efficient ab Initio Method. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 974-987.	5.3	15
11	Generalizing Double-Hybrid Density Functionals: Impact of Higher-Order Perturbation Terms. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 7413-7430.	5.3	12
12	Efficient yet accurate dispersion-corrected semilocal exchange-correlation functionals for non-covalent interactions. <i>Journal of Chemical Physics</i> , 2020, 153, 084117.	3.0	10
13	Improved solid stability from a screened range-separated hybrid functional by satisfying semiclassical atom theory and local density linear response. <i>Physical Review B</i> , 2020, 102, .	3.2	19
14	Improved transition metal surface energies from a generalized gradient approximation developed for quasi two-dimensional systems. <i>Journal of Chemical Physics</i> , 2020, 152, 151101.	3.0	14
15	Screened range-separated hybrid by balancing the compact and slowly varying density regimes: Satisfaction of local density linear response. <i>Journal of Chemical Physics</i> , 2020, 152, 044111.	3.0	22
16	A way of resolving the order-of-limit problem of Tao-Mo semilocal functional. <i>Journal of Chemical Physics</i> , 2020, 153, 184112.	3.0	15
17	Insights from the density functional performance of water and water-solid interactions: SCAN in relation to other meta-GGAs. <i>Journal of Chemical Physics</i> , 2020, 153, 214116.	3.0	14
18	Laplacian free and asymptotic corrected semilocal exchange potential applied to the band gap of solids. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 19639-19650.	2.8	21

#	ARTICLE	IF	CITATIONS
19	Efficient band gap prediction of semiconductors and insulators from a semilocal exchange-correlation functional. <i>Physical Review B</i> , 2019, 100, .	3.2	35
20	Relevance of the Pauli kinetic energy density for semilocal functionals. <i>Physical Review B</i> , 2019, 100, .	3.2	38
21	Performance of Tao-Mo Semilocal Functional with rVV10 Dispersion-Correction: Influence of Different Correlation. <i>Journal of Physical Chemistry A</i> , 2019, 123, 10582-10593.	2.5	14
22	Screened hybrid meta-GGA exchange-correlation functionals for extended systems. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 3002-3015.	2.8	16
23	Improving the Performance of Tao-Mo Non-empirical Density Functional with Broader Applicability in Quantum Chemistry and Materials Science. <i>Journal of Physical Chemistry A</i> , 2019, 123, 6356-6369.	2.5	29
24	Long-range screened hybrid-functional theory satisfying the local-density linear response. <i>Physical Review A</i> , 2019, 99, .	2.5	16
25	A meta-GGA level screened range-separated hybrid functional by employing short range Hartree-Fock with a long range semilocal functional. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 8999-9005.	2.8	21
26	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. <i>Journal of Chemical Physics</i> , 2018, 148, 024111.	3.0	0
27	A Parameter-Free Semilocal Exchange Energy Functional for Two-Dimensional Quantum Systems. <i>Journal of Physical Chemistry A</i> , 2018, 122, 3455-3461.	2.5	5
28	Long-range corrected density functional through the density matrix expansion based semilocal exchange hole. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 8991-8998.	2.8	21
29	Gradient approximated exchange energy functionals with improved performances for two-dimensional quantum dot systems. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2018, 97, 268-276.	2.7	9
30	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. <i>Journal of Chemical Physics</i> , 2018, 149, 164703.	3.0	35
31	On the many-electron self-interaction error of the semilocal exchange hole based meta-GGA level range-separated hybrid with the B88 hybrids. <i>Chemical Physics Letters</i> , 2018, 713, 1-9.	2.6	17
32	Efficient lattice constants and energy bandgaps for condensed systems from a meta-GGA level screened range-separated hybrid functional. <i>Journal of Chemical Physics</i> , 2018, 149, 094105.	3.0	14
33	Assessing the performance of the Tao-Mo semilocal density functional in the projector-augmented-wave method. <i>Journal of Chemical Physics</i> , 2018, 149, 044120.	3.0	50
34	Inhomogeneity induced and appropriately parameterized semilocal exchange and correlation energy functionals in two-dimensions. <i>Journal of Chemical Physics</i> , 2018, 148, 134117.	3.0	5
35	Semilocal Exchange Energy Functional for Two-Dimensional Quantum Systems: A Step Beyond Generalized Gradient Approximations. <i>Journal of Physical Chemistry A</i> , 2017, 121, 4804-4811.	2.5	11
36	Solid-state performance of a meta-GGA screened hybrid density functional constructed from Pauli kinetic enhancement factor dependent semilocal exchange hole. <i>Journal of Chemical Physics</i> , 0, , .	3.0	4