Lucian A Constantin

List of Publications by Year
in descending order

88	12,138	109321 35	48315 88
papers	citations	h-index	g-index

92	92	92	12109
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Restoring the Density-Gradient Expansion for Exchange in Solids and Surfaces. Physical Review Letters, 2008, 100, 136406.	7.8	8,139
2	Workhorse Semilocal Density Functional for Condensed Matter Physics and Quantum Chemistry. Physical Review Letters, 2009, 103, 026403.	7.8	507
3	Some Fundamental Issues in Ground-State Density Functional Theory: A Guide for the Perplexed. Journal of Chemical Theory and Computation, 2009, 5, 902-908.	5.3	306
4	Laplacian-level density functionals for the kinetic energy density and exchange-correlation energy. Physical Review B, 2007, 75, .	3.2	120
5	Semiclassical Neutral Atom as a Reference System in Density Functional Theory. Physical Review Letters, 2011, 106, 186406.	7.8	117
6	Relevance of the Slowly Varying Electron Gas to Atoms, Molecules, and Solids. Physical Review Letters, 2006, 97, 223002.	7.8	94
7	Generalized Gradient Approximations of the Noninteracting Kinetic Energy from the Semiclassical Atom Theory: Rationalization of the Accuracy of the Frozen Density Embedding Theory for Nonbonded Interactions. Journal of Chemical Theory and Computation, 2011, 7, 2439-2451.	5.3	83
8	Kineticâ€energyâ€density dependent semilocal exchangeâ€correlation functionals. International Journal of Quantum Chemistry, 2016, 116, 1641-1694.	2.0	78
9	Meta-generalized gradient approximation for the exchange-correlation hole with an application to the jellium surface energy. Physical Review B, 2006, 73, .	3.2	71
10	High-Level Correlated Approach to the Jellium Surface Energy, without Uniform-Gas Input. Physical Review Letters, 2008, 100, 036401.	7.8	68
11	Semilocal Pauliâ€“Gaussian Kinetic Functionals for Orbital-Free Density Functional Theory Calculations of Solids. Journal of Physical Chemistry Letters, 2018, 9, 4385-4390.	4.6	65
12	Condition on the Kohnâ€“Sham kinetic energy and modern parametrization of the Thomasâ€“Fermi density. Journal of Chemical Physics, 2009, 130, 034107.	3.0	63
13	Optical spectra of solids obtained by time-dependent density functional theory with the jellium-with-gap-model exchange-correlation kernel. Physical Review B, 2013, 87, .	3.2	62
14	Laplacian-Level Kinetic Energy Approximations Based on the Fourth-Order Gradient Expansion: Global Assessment and Application to the Subsystem Formulation of Density Functional Theory. Journal of Chemical Theory and Computation, 2014, 10, 164-179.	5.3	62
15	Meta-GGA Exchange-Correlation Functional with a Balanced Treatment of Nonlocality. Journal of Chemical Theory and Computation, 2013, 9, 2256-2263.	5.3	60
16	PerdewetÂal.Reply:. Physical Review Letters, 2008, 101, .	7.8	59
17	Nonuniform Scaling Applied to Surface Energies of Transition Metals. Physical Review Letters, 2012, 108, 126402.	7.8	57
18	Exchange-correlation hole of a generalized gradient approximation for solids and surfaces. Physical Review B, 2009, 79, .	3.2	54

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19	Semiclassical atom theory applied to solid-state physics. Physical Review B, 2016, 93, .	3.2	51
20	Simple dynamic exchange-correlation kernel of a uniform electron gas. Physical Review B, 2007, 75, .	3.2	50
21	Generalized gradient approximation bridging the rapidly and slowly varying density regimes: A PBE-like functional for hybrid interfaces. Physical Review B, 2010, 82, .	3.2	50
22	Two-Dimensional Scan of the Performance of Generalized Gradient Approximations with Perdewâ€“Burkeâ€“Ernzerhof-Like Enhancement Factor. Journal of Chemical Theory and Computation, 2011, 7, 3548-3559.	5.3	49
23	Kohn-Sham kinetic energy density in the nuclear and asymptotic regions: Deviations from the von WeizsÃcker behavior and applications to density functionals. Physical Review B, 2015, 91, .	3.2	49
24	Semilocal dynamical correlation with increased localization. Physical Review B, 2012, 86, .	3.2	45
25	Laplacian-dependent models of the kinetic energy density: Applications in subsystem density functional theory with meta-generalized gradient approximation functionals. Journal of Chemical Physics, 2017, 146, 064105.	3.0	44
26	Collapse of the Electron Gas to Two Dimensions in Density Functional Theory. Physical Review Letters, 2008, 101, 016406.	7.8	42
27	Relevance of coordinate and particle-number scaling in density-functional theory. Physical Review A, 2013, 87, .	2.5	42
28	Semilocal density functional theory with correct surface asymptotics. Physical Review B, 2016, 93, .	3.2	41
29	Communication: Ionization potentials in the limit of large atomic number. Journal of Chemical Physics, 2010, 133, 241103.	3.0	40
30	Construction of a general semilocal exchange-correlation hole model: Application to nonempirical meta-GGA functionals. Physical Review B, 2013, 88, .	3.2	40
31	Dispersion-corrected PBEsol exchange-correlation functional. Physical Review B, 2018, 98, .	3.2	40
32	Correlation energy functional from jellium surface analysis. Physical Review B, 2011, 84, .	3.2	39
33	Relevance of the Pauli kinetic energy density for semilocal functionals. Physical Review B, 2019, 100, .	3.2	38
34	Performance of Semilocal Kinetic Energy Functionals for Orbital-Free Density Functional Theory. Journal of Chemical Theory and Computation, 2019, 15, 3044-3055.	5.3	37
35	Dimensional crossover of the exchange-correlation energy at the semilocal level. Physical Review B, 2008, 78, .	3.2	36
36	Efficient band gap prediction of semiconductors and insulators from a semilocal exchange-correlation functional. Physical Review B, 2019, 100, .	3.2	35

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37	Exchange-correlation generalized gradient approximation for gold nanostructures. Journal of Chemical Physics, 2011, 134, 194112.	3.0	34
38	Testing the broad applicability of the PBEint GGA functional and its oneâ€parameter hybrid form. International Journal of Quantum Chemistry, 2013, 113, 673-682.	2.0	33
39	Modified Fourth-Order Kinetic Energy Gradient Expansion with Hartree Potential-Dependent Coefficients. Journal of Chemical Theory and Computation, 2017, 13, 4228-4239.	5.3	33
40	Gradient-dependent upper bound for the exchange-correlation energy and application to density functional theory. Physical Review B, 2015, 91, .	3.2	31
41	Nonlocal kinetic energy functional from the jellium-with-gap model: Applications to orbital-free density functional theory. Physical Review B, 2018, 97, .	3.2	31
42	Position-dependent exact-exchange energy for slabs and semi-infinite jellium. Physical Review B, 2009, 80, .	3.2	30
43	Adiabatic-connection-fluctuation-dissipation approach to long-range behavior of exchange-correlation energy at metal surfaces: A numerical study for jellium slabs. Physical Review B, 2011, 83, .	3.2	30
44	Kinetic energy density functionals from the Airy gas with an application to the atomization kinetic energies of molecules. Physical Review B, 2009, 79, .	3.2	28
45	Gradient-dependent exchange-correlation kernel for materials optical properties. Physical Review B, 2018, 98, .	3.2	27
46	Improving atomization energies of molecules and solids with a spin-dependent gradient correction from one-electron density analysis. Physical Review B, 2011, 84, .	3.2	26
47	Simple effective interaction for dimensional crossover. Physical Review B, 2016, 93, .	3.2	26
48	Jellium-with-gap model applied to semilocal kinetic functionals. Physical Review B, 2017, 95, .	3.2	26
49	Wave-vector analysis of the jellium exchange-correlation surface energy in the random-phase approximation: Support for nonempirical density functionals. Physical Review B, 2006, 74, .	3.2	24
50	Spin-dependent gradient correction for more accurate atomization energies of molecules. Journal of Chemical Physics, 2012, 137, 194105.	3.0	23
51	Generalized Gradient Approximation Correlation Energy Functionals Based on the Uniform Electron Gas with Gap Model. Journal of Chemical Theory and Computation, 2014, 10, 2016-2026.	5.3	23
52	Wave Function and Density Functional Theory Studies of Dihydrogen Complexes. Journal of Chemical Theory and Computation, 2014, 10, 3151-3162.	5.3	23
53	Subsystem density functional theory with meta-generalized gradient approximation exchange-correlation functionals. Journal of Chemical Physics, 2015, 142, 154121.	3.0	23
54	Unveiling the Physics Behind Hybrid Functionals. Journal of Physical Chemistry A, 2020, 124, 5606-5614.	2.5	23

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55	Global Hybrids from the Semiclassical Atom Theory Satisfying the Local Density Linear Response. Journal of Chemical Theory and Computation, 2015, 11, 122-131.	5.3	22
56	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
57	Kinetic and Exchange Energy Densities near the Nucleus. Computation, 2016, 4, 19.	2.0	20
58	Correlation energy functionals from adiabatic connection formalism. Physical Review B, 2019, 99, .	3.2	19
59	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
60	Electronic band structure of layers within meta generalized gradient approximation of density functionals. Physical Review B, 2020, 102, .	3.2	18
61	Exchange-correlation energy functional based on the Airy-gas reference system. Physical Review B, 2009, 80, .	3.2	17
62	Solid-State Testing of a Van-Der-Waals-Corrected Exchange-Correlation Functional Based on the Semiclassical Atom Theory. Computation, 2018, 6, 7.	2.0	17
63	Kernel-corrected random-phase approximation for the uniform electron gas and jellium surface energy. Physical Review B, 2016, 94, .	3.2	16
64	Long-range screened hybrid-functional theory satisfying the local-density linear response. Physical Review A, 2019, 99, .	2.5	16
65	Semilocal properties of the Pauli kinetic potential. Physical Review B, 2019, 99, .	3.2	16
66	Hartree potential dependent exchange functional. Journal of Chemical Physics, 2016, 145, 084110.	3.0	15
67	Accurate Water Properties from an Efficient ab Initio Method. Journal of Chemical Theory and Computation, 2020, 16, 974-987.	5.3	15
68	Accurate density functional made more versatile. Journal of Chemical Physics, 2021, 155, 024103.	3.0	15
69	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
70	Modified Interaction-Strength Interpolation Method as an Important Step toward Self-Consistent Calculations. Journal of Chemical Theory and Computation, 2020, 16, 4983-4992.	5.3	14
71	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
72	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

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73	The Role of the Reduced Laplacian Renormalization in the Kinetic Energy Functional Development. Computation, 2019, 7, 65.	2.0	13
74	Nonlocal kinetic energy functionals in real space using a Yukawa-potential kernel: Properties, linear response, and model functionals. Physical Review B, 2021, 103, .	3.2	13
75	Improving the applicability of the Pauli kinetic energy density based semilocal functional for solids. New Journal of Physics, 2021, 23, 063007.	2.9	13
76	Generalizing Double-Hybrid Density Functionals: Impact of Higher-Order Perturbation Terms. Journal of Chemical Theory and Computation, 2020, 16, 7413-7430.	5.3	12
77	Assessment of the TCA functional in computational chemistry and solid-state physics. Theoretical Chemistry Accounts, 2015, 134, 1.	1.4	10
78	Efficient yet accurate dispersion-corrected semilocal exchangeâ€“correlation functionals for non-covalent interactions. Journal of Chemical Physics, 2020, 153, 084117.	3.0	10
79	The Many-Body Exchange-Correlation Hole at Metal Surfaces. Journal of Chemical Theory and Computation, 2009, 5, 895-901.	5.3	8
80	Kinetic Energy Density Functionals Based on a Generalized Screened Coulomb Potential: Linear Response and Future Perspectives. Computation, 2022, 10, 30.	2.0	7
81	Comparison of dispersion-corrected exchange-correlation functionals using atomic orbitals. Physical Review B, 2019, 100, .	3.2	5
82	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
83	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
84	First principles optical spectra of theÎ²-SiC(0â€‰0â€‰1)/Al interface. Journal of Physics Condensed Matter, 2014, 26, 265006.	1.8	3
85	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
86	Quasi-dimensional models applied to kinetic and exchange energy density functionals. European Physical Journal B, 2021, 94, 1.	1.5	0
87	Nonlocal exchange and correlation energy functionals using the Yukawa potential as ingredient: Application to the linear response of the uniform electron gas. Physical Review B, 2021, 104, .	3.2	0
88	Energy Densities of Exchange and Correlation in the Slowly Varying Region of the Airy Gas. Progress in Theoretical Chemistry and Physics, 2009, , 297-310.	0.2	0