

Lucian A Constantin

List of Publications by Citations

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

85
papers

9,180
citations

33
h-index

92
g-index

92
ext. papers

10,621
ext. citations

4
avg, IF

6.11
L-index

#	Paper	IF	Citations
85	Restoring the density-gradient expansion for exchange in solids and surfaces. <i>Physical Review Letters</i> , 2008 , 100, 136406	7.4	5934
84	Workhorse semilocal density functional for condensed matter physics and quantum chemistry. <i>Physical Review Letters</i> , 2009 , 103, 026403	7.4	426
83	Some Fundamental Issues in Ground-State Density Functional Theory: A Guide for the Perplexed. <i>Journal of Chemical Theory and Computation</i> , 2009 , 5, 902-8	6.4	273
82	Semiclassical neutral atom as a reference system in density functional theory. <i>Physical Review Letters</i> , 2011 , 106, 186406	7.4	101
81	Laplacian-level density functionals for the kinetic energy density and exchange-correlation energy. <i>Physical Review B</i> , 2007 , 75,	3.3	100
80	Relevance of the slowly varying electron gas to atoms, molecules, and solids. <i>Physical Review Letters</i> , 2006 , 97, 223002	7.4	83
79	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. <i>Journal of Chemical Theory and Computation</i> , 2011 , 7, 2439-51	6.4	68
78	Meta-generalized gradient approximation for the exchange-correlation hole with an application to the jellium surface energy. <i>Physical Review B</i> , 2006 , 73,	3.3	64
77	High-level correlated approach to the jellium surface energy, without uniform-gas input. <i>Physical Review Letters</i> , 2008 , 100, 036401	7.4	63
76	Kinetic-energy-density dependent semilocal exchange-correlation functionals. <i>International Journal of Quantum Chemistry</i> , 2016 , 116, 1641-1694	2.1	62
75	Condition on the Kohn-Sham kinetic energy and modern parametrization of the Thomas-Fermi density. <i>Journal of Chemical Physics</i> , 2009 , 130, 034107	3.9	56
74	Perdew et al. Reply:. <i>Physical Review Letters</i> , 2008 , 101,	7.4	55
73	Meta-GGA Exchange-Correlation Functional with a Balanced Treatment of Nonlocality. <i>Journal of Chemical Theory and Computation</i> , 2013 , 9, 2256-63	6.4	53
72	Laplacian-Level Kinetic Energy Approximations Based on the Fourth-Order Gradient Expansion: Global Assessment and Application to the Subsystem Formulation of Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 164-79	6.4	52
71	Optical spectra of solids obtained by time-dependent density functional theory with the jellium-with-gap-model exchange-correlation kernel. <i>Physical Review B</i> , 2013 , 87,	3.3	50
70	Nonuniform scaling applied to surface energies of transition metals. <i>Physical Review Letters</i> , 2012 , 108, 126402	7.4	50
69	Semiclassical atom theory applied to solid-state physics. <i>Physical Review B</i> , 2016 , 93,	3.3	49

68	Two-Dimensional Scan of the Performance of Generalized Gradient Approximations with Perdew-Burke-Ernzerhof-Like Enhancement Factor. <i>Journal of Chemical Theory and Computation</i> , 2011 , 7, 3548-59	6.4	46
67	Generalized gradient approximation bridging the rapidly and slowly varying density regimes: A PBE-like functional for hybrid interfaces. <i>Physical Review B</i> , 2010 , 82,	3.3	46
66	Kohn-Sham kinetic energy density in the nuclear and asymptotic regions: Deviations from the von Weizsäcker behavior and applications to density functionals. <i>Physical Review B</i> , 2015 , 91,	3.3	44
65	Simple dynamic exchange-correlation kernel of a uniform electron gas. <i>Physical Review B</i> , 2007 , 75,	3.3	43
64	Semilocal Pauli-Gaussian Kinetic Functionals for Orbital-Free Density Functional Theory Calculations of Solids. <i>Journal of Physical Chemistry Letters</i> , 2018 , 9, 4385-4390	6.4	42
63	Exchange-correlation hole of a generalized gradient approximation for solids and surfaces. <i>Physical Review B</i> , 2009 , 79,	3.3	42
62	Collapse of the electron gas to two dimensions in density functional theory. <i>Physical Review Letters</i> , 2008 , 101, 016406	7.4	41
61	Semilocal dynamical correlation with increased localization. <i>Physical Review B</i> , 2012 , 86,	3.3	39
60	Construction of a general semilocal exchange-correlation hole model: Application to nonempirical meta-GGA functionals. <i>Physical Review B</i> , 2013 , 88,	3.3	37
59	Laplacian-dependent models of the kinetic energy density: Applications in subsystem density functional theory with meta-generalized gradient approximation functionals. <i>Journal of Chemical Physics</i> , 2017 , 146, 064105	3.9	36
58	Semilocal density functional theory with correct surface asymptotics. <i>Physical Review B</i> , 2016 , 93,	3.3	36
57	Correlation energy functional from jellium surface analysis. <i>Physical Review B</i> , 2011 , 84,	3.3	36
56	Communication: Ionization potentials in the limit of large atomic number. <i>Journal of Chemical Physics</i> , 2010 , 133, 241103	3.9	35
55	Relevance of coordinate and particle-number scaling in density-functional theory. <i>Physical Review A</i> , 2013 , 87,	2.6	34
54	Exchange-correlation generalized gradient approximation for gold nanostructures. <i>Journal of Chemical Physics</i> , 2011 , 134, 194112	3.9	33
53	Dimensional crossover of the exchange-correlation energy at the semilocal level. <i>Physical Review B</i> , 2008 , 78,	3.3	32
52	Testing the broad applicability of the PBEint GGA functional and its one-parameter hybrid form. <i>International Journal of Quantum Chemistry</i> , 2013 , 113, 673-682	2.1	29
51	Adiabatic-connection-fluctuation-dissipation approach to long-range behavior of exchange-correlation energy at metal surfaces: A numerical study for jellium slabs. <i>Physical Review B</i> , 2011 , 83,	3.3	29

50	Gradient-dependent upper bound for the exchange-correlation energy and application to density functional theory. <i>Physical Review B</i> , 2015 , 91,	3.3	28
49	Dispersion-corrected PBEsol exchange-correlation functional. <i>Physical Review B</i> , 2018 , 98,	3.3	26
48	Efficient band gap prediction of semiconductors and insulators from a semilocal exchange-correlation functional. <i>Physical Review B</i> , 2019 , 100,	3.3	24
47	Modified Fourth-Order Kinetic Energy Gradient Expansion with Hartree Potential-Dependent Coefficients. <i>Journal of Chemical Theory and Computation</i> , 2017 , 13, 4228-4239	6.4	24
46	Kinetic energy density functionals from the Airy gas with an application to the atomization kinetic energies of molecules. <i>Physical Review B</i> , 2009 , 79,	3.3	24
45	Relevance of the Pauli kinetic energy density for semilocal functionals. <i>Physical Review B</i> , 2019 , 100,	3.3	23
44	Improving atomization energies of molecules and solids with a spin-dependent gradient correction from one-electron density analysis. <i>Physical Review B</i> , 2011 , 84,	3.3	23
43	Position-dependent exact-exchange energy for slabs and semi-infinite jellium. <i>Physical Review B</i> , 2009 , 80,	3.3	22
42	Wave-vector analysis of the jellium exchange-correlation surface energy in the random-phase approximation: Support for nonempirical density functionals. <i>Physical Review B</i> , 2006 , 74,	3.3	22
41	Jellium-with-gap model applied to semilocal kinetic functionals. <i>Physical Review B</i> , 2017 , 95,	3.3	21
40	Subsystem density functional theory with meta-generalized gradient approximation exchange-correlation functionals. <i>Journal of Chemical Physics</i> , 2015 , 142, 154121	3.9	21
39	Wave Function and Density Functional Theory Studies of Dihydrogen Complexes. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 3151-62	6.4	21
38	Spin-dependent gradient correction for more accurate atomization energies of molecules. <i>Journal of Chemical Physics</i> , 2012 , 137, 194105	3.9	21
37	Nonlocal kinetic energy functional from the jellium-with-gap model: Applications to orbital-free density functional theory. <i>Physical Review B</i> , 2018 , 97,	3.3	20
36	Global hybrids from the semiclassical atom theory satisfying the local density linear response. <i>Journal of Chemical Theory and Computation</i> , 2015 , 11, 122-31	6.4	20
35	Simple effective interaction for dimensional crossover. <i>Physical Review B</i> , 2016 , 93,	3.3	19
34	Performance of Semilocal Kinetic Energy Functionals for Orbital-Free Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2019 , 15, 3044-3055	6.4	18
33	Gradient-dependent exchange-correlation kernel for materials optical properties. <i>Physical Review B</i> , 2018 , 98,	3.3	18

32	Kinetic and Exchange Energy Densities near the Nucleus. <i>Computation</i> , 2016 , 4, 19	2.2	18
31	Generalized Gradient Approximation Correlation Energy Functionals Based on the Uniform Electron Gas with Gap Model. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 2016-26	6.4	17
30	Exchange-correlation energy functional based on the Airy-gas reference system. <i>Physical Review B</i> , 2009 , 80,	3.3	15
29	Solid-State Testing of a Van-Der-Waals-Corrected Exchange-Correlation Functional Based on the Semiclassical Atom Theory. <i>Computation</i> , 2018 , 6, 7	2.2	14
28	Unveiling the Physics Behind Hybrid Functionals. <i>Journal of Physical Chemistry A</i> , 2020 , 124, 5606-5614	2.8	13
27	Kernel-corrected random-phase approximation for the uniform electron gas and jellium surface energy. <i>Physical Review B</i> , 2016 , 94,	3.3	13
26	Accurate Water Properties from an Efficient ab Initio Method. <i>Journal of Chemical Theory and Computation</i> , 2020 , 16, 974-987	6.4	12
25	Correlation energy functionals from adiabatic connection formalism. <i>Physical Review B</i> , 2019 , 99,	3.3	12
24	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	3.9	11
23	Long-range screened hybrid-functional theory satisfying the local-density linear response. <i>Physical Review A</i> , 2019 , 99,	2.6	10
22	Semilocal properties of the Pauli kinetic potential. <i>Physical Review B</i> , 2019 , 99,	3.3	10
21	Electronic band structure of layers within meta generalized gradient approximation of density functionals. <i>Physical Review B</i> , 2020 , 102,	3.3	10
20	Hartree potential dependent exchange functional. <i>Journal of Chemical Physics</i> , 2016 , 145, 084110	3.9	10
19	The Role of the Reduced Laplacian Renormalization in the Kinetic Energy Functional Development. <i>Computation</i> , 2019 , 7, 65	2.2	9
18	Assessment of the TCA functional in computational chemistry and solid-state physics. <i>Theoretical Chemistry Accounts</i> , 2015 , 134, 1	1.9	8
17	Efficient yet accurate dispersion-corrected semilocal exchange-correlation functionals for non-covalent interactions. <i>Journal of Chemical Physics</i> , 2020 , 153, 084117	3.9	8
16	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,	3.3	7
15	Generalizing Double-Hybrid Density Functionals: Impact of Higher-Order Perturbation Terms. <i>Journal of Chemical Theory and Computation</i> , 2020 , 16, 7413-7430	6.4	7

14	The Many-Body Exchange-Correlation Hole at Metal Surfaces. <i>Journal of Chemical Theory and Computation</i> , 2009 , 5, 895-901	6.4	6
13	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	3.9	6
12	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	3.9	5
11	Modified Interaction-Strength Interpolation Method as an Important Step toward Self-Consistent Calculations. <i>Journal of Chemical Theory and Computation</i> , 2020 , 16, 4983-4992	6.4	5
10	Comparison of dispersion-corrected exchange-correlation functionals using atomic orbitals. <i>Physical Review B</i> , 2019 , 100,	3.3	4
9	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	3.8	4
8	First principles optical spectra of the BiC(0 0 1)/Al interface. <i>Journal of Physics Condensed Matter</i> , 2014 , 26, 265006	1.8	3
7	Nonlocal kinetic energy functionals in real space using a Yukawa-potential kernel: Properties, linear response, and model functionals. <i>Physical Review B</i> , 2021 , 103,	3.3	3
6	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	3
5	Accurate density functional made more versatile. <i>Journal of Chemical Physics</i> , 2021 , 155, 024103	3.9	3
4	Kinetic Energy Density Functionals Based on a Generalized Screened Coulomb Potential: Linear Response and Future Perspectives. <i>Computation</i> , 2022 , 10, 30	2.2	1
3	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	3.9	0
2	Energy Densities of Exchange and Correlation in the Slowly Varying Region of the Airy Gas. <i>Progress in Theoretical Chemistry and Physics</i> , 2009 , 297-310	0.6	
1	Quasi-dimensional models applied to kinetic and exchange energy density functionals. <i>European Physical Journal B</i> , 2021 , 94, 1	1.2	