Lucian A Constantin

List of Publications by Year in Descending Order

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	Kinetic Energy Density Functionals Based on a Generalized Screened Coulomb Potential: Linear Response and Future Perspectives. *Computation*, **2022**, 10, 30	2.2	1
84	Nonlocal kinetic energy functionals in real space using a Yukawa-potential kernel: Properties, linear response, and model functionals. *Physical Review B*, **2021**, 103,	3.3	3
83	Improving the applicability of the Pauli kinetic energy density based semilocal functional for solids. *New Journal of Physics*, **2021**, 23, 063007	2.9	3
82	Quasi-dimensional models applied to kinetic and exchange energy density functionals. *European Physical Journal B*, **2021**, 94, 1	1.2	
81	Correct Structural Phase Stability of FeS2, TiO2, and MnO2 from a Semilocal Density Functional. *Journal of Physical Chemistry C*, **2021**, 125, 4284-4291	3.8	4
80	Accurate density functional made more versatile. *Journal of Chemical Physics*, **2021**, 155, 024103	3.9	3
79	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	3.9	0
78	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,	3.3	7
77	Improved transition metal surface energies from a generalized gradient approximation developed for quasi two-dimensional systems. *Journal of Chemical Physics*, **2020**, 152, 151101	3.9	5
76	Unveiling the Physics Behind Hybrid Functionals. *Journal of Physical Chemistry A*, **2020**, 124, 5606-5614	2.8	13
75	Modified Interaction-Strength Interpolation Method as an Important Step toward Self-Consistent Calculations. *Journal of Chemical Theory and Computation*, **2020**, 16, 4983-4992	6.4	5
74	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	3.9	11
73	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	3.9	6
72	Accurate Water Properties from an Efficient ab Initio Method. *Journal of Chemical Theory and Computation*, **2020**, 16, 974-987	6.4	12
71	Generalizing Double-Hybrid Density Functionals: Impact of Higher-Order Perturbation Terms. *Journal of Chemical Theory and Computation*, **2020**, 16, 7413-7430	6.4	7
70	Electronic band structure of layers within meta generalized gradient approximation of density functionals. *Physical Review B*, **2020**, 102,	3.3	10
69	Efficient yet accurate dispersion-corrected semilocal exchange-correlation functionals for non-covalent interactions. *Journal of Chemical Physics*, **2020**, 153, 084117	3.9	8

68	Long-range screened hybrid-functional theory satisfying the local-density linear response. *Physical Review A*, **2019**, 99,	2.6	10
67	Semilocal properties of the Pauli kinetic potential. *Physical Review B*, **2019**, 99,	3.3	10
66	Performance of Semilocal Kinetic Energy Functionals for Orbital-Free Density Functional Theory. *Journal of Chemical Theory and Computation*, **2019**, 15, 3044-3055	6.4	18
65	Efficient band gap prediction of semiconductors and insulators from a semilocal exchange-correlation functional. *Physical Review B*, **2019**, 100,	3.3	24
64	Relevance of the Pauli kinetic energy density for semilocal functionals. *Physical Review B*, **2019**, 100,	3.3	23
63	Correlation energy functionals from adiabatic connection formalism. *Physical Review B*, **2019**, 99,	3.3	12
62	The Role of the Reduced Laplacian Renormalization in the Kinetic Energy Functional Development. *Computation*, **2019**, 7, 65	2.2	9
61	Comparison of dispersion-corrected exchange-correlation functionals using atomic orbitals. *Physical Review B*, **2019**, 100,	3.3	4
60	Nonlocal kinetic energy functional from the jellium-with-gap model: Applications to orbital-free density functional theory. *Physical Review B*, **2018**, 97,	3.3	20
59	Semilocal Pauli-Gaussian Kinetic Functionals for Orbital-Free Density Functional Theory Calculations of Solids. *Journal of Physical Chemistry Letters*, **2018**, 9, 4385-4390	6.4	42
58	Solid-State Testing of a Van-Der-Waals-Corrected Exchange-Correlation Functional Based on the Semiclassical Atom Theory. *Computation*, **2018**, 6, 7	2.2	14
57	Gradient-dependent exchange-correlation kernel for materials optical properties. *Physical Review B* , **2018**, 98,	3.3	18
56	Dispersion-corrected PBEsol exchange-correlation functional. *Physical Review B*, **2018**, 98,	3.3	26
55	Jellium-with-gap model applied to semilocal kinetic functionals. *Physical Review B*, **2017**, 95,	3.3	21
54	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	3.9	36
53	Modified Fourth-Order Kinetic Energy Gradient Expansion with Hartree Potential-Dependent Coefficients. *Journal of Chemical Theory and Computation*, **2017**, 13, 4228-4239	6.4	24
52	Kinetic-energy-density dependent semilocal exchange-correlation functionals. *International Journal of Quantum Chemistry*, **2016**, 116, 1641-1694	2.1	62
51	Semiclassical atom theory applied to solid-state physics. *Physical Review B*, **2016**, 93,	3.3	49

50	Semilocal density functional theory with correct surface asymptotics. *Physical Review B*, **2016**, 93,	3.3	36
49	Simple effective interaction for dimensional crossover. *Physical Review B*, **2016**, 93,	3.3	19
48	Kernel-corrected random-phase approximation for the uniform electron gas and jellium surface energy. *Physical Review B*, **2016**, 94,	3.3	13
47	Kinetic and Exchange Energy Densities near the Nucleus. *Computation*, **2016**, 4, 19	2.2	18
46	Hartree potential dependent exchange functional. *Journal of Chemical Physics*, **2016**, 145, 084110	3.9	10
45	Gradient-dependent upper bound for the exchange-correlation energy and application to density functional theory. *Physical Review B*, **2015**, 91,	3.3	28
44	Kohn-Sham kinetic energy density in the nuclear and asymptotic regions: Deviations from the von Weizs□ker behavior and applications to density functionals. *Physical Review B*, **2015**, 91,	3.3	44
43	Assessment of the TCA functional in computational chemistry and solid-state physics. *Theoretical Chemistry Accounts*, **2015**, 134, 1	1.9	8
42	Subsystem density functional theory with meta-generalized gradient approximation exchange-correlation functionals. *Journal of Chemical Physics*, **2015**, 142, 154121	3.9	21
41	Global hybrids from the semiclassical atom theory satisfying the local density linear response. *Journal of Chemical Theory and Computation*, **2015**, 11, 122-31	6.4	20
40	Generalized Gradient Approximation Correlation Energy Functionals Based on the Uniform Electron Gas with Gap Model. *Journal of Chemical Theory and Computation*, **2014**, 10, 2016-26	6.4	17
39	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, 164-79	6.4	52
38	Wave Function and Density Functional Theory Studies of Dihydrogen Complexes. *Journal of Chemical Theory and Computation*, **2014**, 10, 3151-62	6.4	21
37	First principles optical spectra of the □SiC(0 0 1)/Al interface. *Journal of Physics Condensed Matter*, **2014**, 26, 265006	1.8	3
36	Testing the broad applicability of the PBEint GGA functional and its one-parameter hybrid form. *International Journal of Quantum Chemistry*, **2013**, 113, 673-682	2.1	29
35	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,	3.3	50
34	Meta-GGA Exchange-Correlation Functional with a Balanced Treatment of Nonlocality. *Journal of Chemical Theory and Computation*, **2013**, 9, 2256-63	6.4	53
33	Relevance of coordinate and particle-number scaling in density-functional theory. *Physical Review A* , **2013**, 87,	2.6	34

32	Construction of a general semilocal exchange-correlation hole model: Application to nonempirical meta-GGA functionals. *Physical Review B*, **2013**, 88,	3.3	37
31	Spin-dependent gradient correction for more accurate atomization energies of molecules. *Journal of Chemical Physics*, **2012**, 137, 194105	3.9	21
30	Nonuniform scaling applied to surface energies of transition metals. *Physical Review Letters*, **2012**, 108, 126402	7.4	50
29	Semilocal dynamical correlation with increased localization. *Physical Review B*, **2012**, 86,	3.3	39
28	Two-Dimensional Scan of the Performance of Generalized Gradient Approximations with Perdew-Burke-Ernzerhof-Like Enhancement Factor. *Journal of Chemical Theory and Computation*, **2011**, 7, 3548-59	6.4	46
27	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, 2439-51	6.4	68
26	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,	3.3	29
25	Semiclassical neutral atom as a reference system in density functional theory. *Physical Review Letters*, **2011**, 106, 186406	7.4	101
24	Improving atomization energies of molecules and solids with a spin-dependent gradient correction from one-electron density analysis. *Physical Review B*, **2011**, 84,	3.3	23
23	Correlation energy functional from jellium surface analysis. *Physical Review B*, **2011**, 84,	3.3	36
22	Exchange-correlation generalized gradient approximation for gold nanostructures. *Journal of Chemical Physics*, **2011**, 134, 194112	3.9	33
21	Generalized gradient approximation bridging the rapidly and slowly varying density regimes: A PBE-like functional for hybrid interfaces. *Physical Review B*, **2010**, 82,	3.3	46
20	Communication: Ionization potentials in the limit of large atomic number. *Journal of Chemical Physics*, **2010**, 133, 241103	3.9	35
19	Exchange-correlation energy functional based on the Airy-gas reference system. *Physical Review B*, **2009**, 80,	3.3	15
18	Exchange-correlation hole of a generalized gradient approximation for solids and surfaces. *Physical Review B*, **2009**, 79,	3.3	42
17	Kinetic energy density functionals from the Airy gas with an application to the atomization kinetic energies of molecules. *Physical Review B*, **2009**, 79,	3.3	24
16	Condition on the Kohn-Sham kinetic energy and modern parametrization of the Thomas-Fermi density. *Journal of Chemical Physics*, **2009**, 130, 034107	3.9	56
15	The Many-Body Exchange-Correlation Hole at Metal Surfaces. *Journal of Chemical Theory and Computation*, **2009**, 5, 895-901	6.4	6

14	Some Fundamental Issues in Ground-State Density Functional Theory: A Guide for the Perplexed. *Journal of Chemical Theory and Computation*, **2009**, 5, 902-8	6.4	273
13	Workhorse semilocal density functional for condensed matter physics and quantum chemistry. *Physical Review Letters*, **2009**, 103, 026403	7.4	426
12	Position-dependent exact-exchange energy for slabs and semi-infinite jellium. *Physical Review B*, **2009**, 80,	3.3	22
11	Energy Densities of Exchange and Correlation in the Slowly Varying Region of the Airy Gas. *Progress in Theoretical Chemistry and Physics*, **2009**, 297-310	0.6	
10	Perdew et al. Reply:. *Physical Review Letters*, **2008**, 101,	7.4	55
9	Collapse of the electron gas to two dimensions in density functional theory. *Physical Review Letters*, **2008**, 101, 016406	7.4	41
8	Dimensional crossover of the exchange-correlation energy at the semilocal level. *Physical Review B*, **2008**, 78,	3.3	32
7	High-level correlated approach to the jellium surface energy, without uniform-gas input. *Physical Review Letters*, **2008**, 100, 036401	7.4	63
6	Restoring the density-gradient expansion for exchange in solids and surfaces. *Physical Review Letters*, **2008**, 100, 136406	7.4	5934
5	Simple dynamic exchange-correlation kernel of a uniform electron gas. *Physical Review B*, **2007**, 75,	3.3	43
4	Laplacian-level density functionals for the kinetic energy density and exchange-correlation energy. *Physical Review B*, **2007**, 75,	3.3	100
3	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,	3.3	22
2	Relevance of the slowly varying electron gas to atoms, molecules, and solids. *Physical Review Letters*, **2006**, 97, 223002	7.4	83
1	Meta-generalized gradient approximation for the exchange-correlation hole with an application to the jellium surface energy. *Physical Review B*, **2006**, 73,	3.3	64