Mel Levy

List of Publications by Citations

77 papers	11,671 citations	31 h-index	80 g-index
80 ext. papers	12,428 ext. citations	3.2 avg, IF	6.02 L-index

#	Paper	IF	Citations
77	Electronegativity: The density functional viewpoint. *Journal of Chemical Physics*, **1978**, 68, 3801-3807	3.9	2329
76	Density-Functional Theory for Fractional Particle Number: Derivative Discontinuities of the Energy. *Physical Review Letters*, **1982**, 49, 1691-1694	7.4	2236
75	Physical Content of the Exact Kohn-Sham Orbital Energies: Band Gaps and Derivative Discontinuities. *Physical Review Letters*, **1983**, 51, 1884-1887	7.4	1795
74	Hellmann-Feynman, virial, and scaling requisites for the exact universal density functionals. Shape of the correlation potential and diamagnetic susceptibility for atoms. *Physical Review A*, **1985**, 32, 2010-2021	2.6	814
73	Exact differential equation for the density and ionization energy of a many-particle system. *Physical Review A*, **1984**, 30, 2745-2748	2.6	713
72	Electron densities in search of Hamiltonians. *Physical Review A*, **1982**, 26, 1200-1208	2.6	502
71	Exact Kohn-Sham scheme based on perturbation theory. *Physical Review A*, **1994**, 50, 196-204	2.6	468
70	Perspective on Density functional approach to the frontier-electron theory of chemical reactivity *Theoretical Chemistry Accounts*, **2000**, 103, 353-360	1.9	374
69	Correlation-energy functional and its high-density limit obtained from a coupling-constant perturbation expansion. *Physical Review B*, **1993**, 47, 13105-13113	3.3	354
68	Density-functional exchange correlation through coordinate scaling in adiabatic connection and correlation hole. *Physical Review A*, **1991**, 43, 4637-4646	2.6	241
67	Variational Density-Functional Theory for an Individual Excited State. *Physical Review Letters*, **1999**, 83, 4361-4364	7.4	167
66	DFT ionization formulas and a DFT perturbation theory for exchange and correlation, through adiabatic connection. *International Journal of Quantum Chemistry*, **1995**, 56, 93-108	2.1	136
65	Strictly correlated electrons in density-functional theory. *Physical Review A*, **1999**, 59, 51-54	2.6	123
64	Hybrid schemes combining the Hartree Fock method and density-functional theory: Underlying formalism and properties of correlation functionals. *Journal of Chemical Physics*, **1997**, 106, 2675-2680	3.9	85
63	Generalized density-functional theory: Conquering the N-representability problem with exact functionals for the electron pair density and the second-order reduced density matrix. *Journal of Chemical Sciences*, **2005**, 117, 507-514	1.8	70
62	Correlation-energy density-functional formulas from correlating first-order density matrices. *Physical Review A*, **1995**, 52, R1808-R1810	2.6	70
61	Relation between exchange-only optimized potential and Kohn-Sham methods with finite basis sets, and effect of linearly dependent products of orbital basis functions. *Journal of Chemical Physics*, **2008**, 128, 104104	3.9	57

60	Density functionals for exchange and correlation energies: Exact conditions and comparison of approximations. *International Journal of Quantum Chemistry*, **1994**, 49, 539-548	2.1	53
59	Exact high-density limit of correlation potential for two-electron density. *Journal of Chemical Physics*, **1999**, 110, 10262-10268	3.9	49
58	Line-integral formulas for exchange and correlation potentials separately. *Physical Review A*, **1997**, 55, 1885-1889	2.6	47
57	Direct first principles algorithm for the universal electron density functional. *Journal of Chemical Physics*, **1982**, 77, 396-398	3.9	47
56	Approximate noninteracting kinetic energy functionals from a nonuniform scaling requirement. *International Journal of Quantum Chemistry*, **1991**, 40, 379-388	2.1	46
55	Expectation values in density-functional theory, and kinetic contribution to the exchange-correlation energy. *Physical Review B*, **1993**, 47, 1167-1173	3.3	45
54	A new functional with homogeneous coordinate scaling in density functional theory: F [□] *Journal of Chemical Physics*, **1985**, 83, 2334-2336	3.9	44
53	Time-independent density-functional theory for excited states of Coulomb systems. *Physical Review A*, **2012**, 85,	2.6	41
52	Time-independent (static) density-functional theories for pure excited states: Extensions and unification. *Physical Review A*, **2009**, 80,	2.6	40
51	Density-functional exchange identity from coordinate scaling. *Physical Review A*, **1996**, 53, 3140-3142	2.6	40
50	An energy-density equation for isoelectronic changes in atoms. *Journal of Chemical Physics*, **1978**, 68, 5298-5299	3.9	36
49	Sum rules for exchange and correlation potentials. *Journal of Chemical Physics*, **2001**, 115, 4438-4443	3.9	35
48	Atomic binding energies from fundamental theorems involving the electron density, <r□>, and the Z□ perturbation expansion. *Journal of Chemical Physics*, **1980**, 72, 3416-3417	3.9	35
47	Rigorous and approximate relations between expectation values of atoms. *Journal of Chemical Physics*, **1980**, 72, 4009-4013	3.9	34
46	Ground-state energy as a simple sum of orbital energies in Kohn-Sham theory: a shift in perspective through a shift in potential. *Physical Review Letters*, **2014**, 113, 113002	7.4	30
45	Success of quantum mechanical approximations for molecular geometries and electron□nuclear attraction expectation values: Gift of the Coulomb potential?. *Journal of Chemical Physics*, **1986**, 84, 4519-4523	3.9	30
44	Average local ionization energies in the Hartree-Fock and Kohn-Sham theories. *Journal of Physical Chemistry A*, **2009**, 113, 1384-9	2.8	29
43	Recent constrained-search advances for approximating density functionals. *The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties*, **1994**, 69, 763-769		29

42	A discontinuous energy–density functional. *Journal of Chemical Physics*, **1982**, 77, 3140-3147	3.9	27
41	Connections between ground-state energies from optimized-effective potential exchange-only and Hartree–Fock methods. *Journal of Chemical Physics*, **2003**, 119, 7087-7093	3.9	26
40	Electron density-functional theory and x-ray structure factors. *Physical Review B*, **1987**, 35, 7887-7890	3.3	26
39	Accurate correlation potentials from integral formulation of density functional perturbation theory. *Journal of Chemical Physics*, **2002**, 116, 6924-6929	3.9	23
38	Method for direct determination of localized orbitals. *Journal of Chemical Physics*, **1975**, 63, 316-318	3.9	23
37	On approximate energy differences from average electron densities. *Journal of Chemical Physics*, **1979**, 70, 1573-1574	3.9	22
36	Energy-density relations and screening constants in atoms. *Journal of Chemical Physics*, **1980**, 73, 5168-5173	3.9	21
35	On the simple constrained-search reformulation of the Hohenberg–Kohn theorem to include degeneracies and more (1964–1979). *International Journal of Quantum Chemistry*, **2010**, 110, 3140-3144	2.1	20
34	Connections between High-Density Scaling Limits of DFT Correlation Energies and Second-Order Z-1 Quantum Chemistry Correlation Energy. *Journal of Physical Chemistry A*, **1998**, 102, 3151-3156	2.8	18
33	Improving energies by using exact electron densities. *Physical Review A*, **1996**, 53, R2915-R2917	2.6	18
32	Comment on "Functional derivative of the universal density functional in Fock space". *Physical Review A*, **2009**, 79,	2.6	16
31	Bounds for the exchange and correlation potentials. *Physical Review A*, **1995**, 51, 2851-2856	2.6	15
30	Augmented potential, energy densities, and virial relations in the weak- and strong-interaction limits of DFT. *Journal of Chemical Physics*, **2017**, 147, 214107	3.9	14
29	Asymptotic coordinate scaling bound for exchange-correlation energy in density-functional theory. *International Journal of Quantum Chemistry*, **2009**, 36, 617-619	2.1	12
28	Unconstrained exchange localization and distant orbital tails. *Journal of Chemical Physics*, **1976**, 65, 2473-2475	3.9	11
27	Formal expressions and corresponding expansions for the exact Kohn-Sham exchange potential. *Physical Review A*, **2009**, 80,	2.6	10
26	Approach to density-functional ionization energy. *Physical Review B*, **1996**, 53, 969-972	3.3	10
25	Energy differences from electrostatic potentials at nuclei. *Journal of Chemical Physics*, **1987**, 87, 5044-5046	3.9	10

24	The nearest self-adjoint operator. *Journal of Chemical Physics*, **1980**, 72, 780-781	3.9	10
23	Mathematical thoughts in DFT. *International Journal of Quantum Chemistry*, **2016**, 116, 802-804	2.1	10
22	Kinetic and electron-electron energies for convex sums of ground state densities with degeneracies and fractional electron number. *Journal of Chemical Physics*, **2014**, 140, 18A538	3.9	9
21	Kinetic energy from a single Kohn-Sham orbital. *Physical Review A*, **2009**, 79,	2.6	9
20	New exact relations for improving the exchange and correlation potentials. *International Journal of Quantum Chemistry*, **1995**, 56, 385-388	2.1	8
19	Exact local exchange potential from Fock equations at vanishing coupling constant, and delta Tc/ delta n from wave-function calculations at full coupling constant. *Physical Review A*, **1996**, 53, 3963-3965	2.6	8
18	Closed-form expression relating the second-order component of the density functional theory correlation energy to its functional derivative. *Journal of Chemical Physics*, **1998**, 109, 6280-6286	3.9	7
17	Adiabatic integration formula for the correlation energy functional of the Hartree□Fock density. *Theoretical Chemistry Accounts*, **1999**, 103, 117-123	1.9	6
16	Variational energy functionals involving one-electron operators. *Journal of Chemical Physics*, **1977**, 67, 724-726	3.9	6
15	Highly Excited States from a Time Independent Density Functional Method. *Computation*, **2016**, 4, 28	2.2	6
14	On augmented Kohn□Sham potential for energy as a simple sum of orbital energies. *Molecular Physics*, **2016**, 114, 1162-1164	1.7	5
13	Tight constraints on the exchange-correlation potentials of degenerate states. *Journal of Chemical Physics*, **2014**, 140, 18A537	3.9	5
12	Nodal variational principle for excited states. *Physical Review A*, **2018**, 98,	2.6	4
11	Approximating the Shifted Hartree-Exchange-Correlation Potential in Direct Energy Kohn-Sham Theory. *Journal of Chemical Theory and Computation*, **2018**, 14, 684-692	6.4	3
10	Additive density functional correlation corrections to single particle theories. *International Journal of Quantum Chemistry*, **1997**, 61, 281-285	2.1	3
9	Simple hydrogenic estimates for the exchange and correlation energies of atoms and atomic ions, with implications for density functional theory. *Journal of Chemical Physics*, **2020**, 153, 074114	3.9	3
8	Properties of Augmented Kohn-Sham Potential for Energy as Simple Sum of Orbital Energies. *Journal of Physical Chemistry A*, **2017**, 121, 342-347	2.8	2
7	On the best partitioning of the density functional energy. *Journal of Molecular Modeling*, **2018**, 24, 311	2	0

6	Generalized Variational Theorem in Quantum Mechanics **2015**, 92-97	
5	Pointwise and generalized virial theorems. *International Journal of Quantum Chemistry*, **2009**, 14, 343-344	1.1
4	Properties of the exact universal density and one-matrix functionals. *International Journal of Quantum Chemistry*, **2009**, 28, 743-744	2.1
3	THEOREMS FOR EXACT LOCAL EXCHANGE POTENTIAL. *Modern Physics Letters B*, **1991**, 05, 1613-1616	1.6
2	Line-integral formulas for exchange and correlation potentials separately. *World Scientific Series in 20th Century Physics*, **2009**, 613-617	0
1	On the adiabatic connection method, and scaling of electron–electron interactions in the Thomas–Fermi limit. *World Scientific Series in 20th Century Physics*, **2009**, 542-545	0