

# Mel Levy

## List of Publications by Year in descending order

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78  
papers

13,402  
citations

136740

32  
h-index

79541

73  
g-index

80  
all docs

80  
docs citations

80  
times ranked

6591  
citing authors

#	ARTICLE	IF	CITATIONS
1	Electronegativity: The density functional viewpoint. <i>Journal of Chemical Physics</i> , 1978, 68, 3801-3807.	1.2	2,806
2	Density-Functional Theory for Fractional Particle Number: Derivative Discontinuities of the Energy. <i>Physical Review Letters</i> , 1982, 49, 1691-1694.	2.9	2,573
3	Physical Content of the Exact Kohn-Sham Orbital Energies: Band Gaps and Derivative Discontinuities. <i>Physical Review Letters</i> , 1983, 51, 1884-1887.	2.9	2,105
4	Hellmann-Feynman, virial, and scaling requisites for the exact universal density functionals. Shape of the correlation potential and diamagnetic susceptibility for atoms. <i>Physical Review A</i> , 1985, 32, 2010-2021.	1.0	897
5	Exact differential equation for the density and ionization energy of a many-particle system. <i>Physical Review A</i> , 1984, 30, 2745-2748.	1.0	803
6	Electron densities in search of Hamiltonians. <i>Physical Review A</i> , 1982, 26, 1200-1208.	1.0	570
7	Exact Kohn-Sham scheme based on perturbation theory. <i>Physical Review A</i> , 1994, 50, 196-204.	1.0	506
8	Perspective on "Density functional approach to the frontier-electron theory of chemical reactivity". <i>Theoretical Chemistry Accounts</i> , 2000, 103, 353-360.	0.5	424
9	Correlation-energy functional and its high-density limit obtained from a coupling-constant perturbation expansion. <i>Physical Review B</i> , 1993, 47, 13105-13113.	1.1	385
10	Density-functional exchange correlation through coordinate scaling in adiabatic connection and correlation hole. <i>Physical Review A</i> , 1991, 43, 4637-4646.	1.0	261
11	Variational Density-Functional Theory for an Individual Excited State. <i>Physical Review Letters</i> , 1999, 83, 4361-4364.	2.9	180
12	Strictly correlated electrons in density-functional theory. <i>Physical Review A</i> , 1999, 59, 51-54.	1.0	146
13	DFT ionization formulas and aDFT perturbation theory for exchange and correlation, through adiabatic connection. <i>International Journal of Quantum Chemistry</i> , 1995, 56, 93-108.	1.0	142
14	Correlation-energy density-functional formulas from correlating first-order density matrices. <i>Physical Review A</i> , 1995, 52, R1808-R1810.	1.0	98
15	Hybrid schemes combining the Hartree-Fock method and density-functional theory: Underlying formalism and properties of correlation functionals. <i>Journal of Chemical Physics</i> , 1997, 106, 2675-2680.	1.2	97
16	Generalized density-functional theory: Conquering the N-representability problem with exact functionals for the electron pair density and the second-order reduced density matrix. <i>Journal of Chemical Sciences</i> , 2005, 117, 507-514.	0.7	79
17	Relation between exchange-only optimized potential and Kohn-Sham methods with finite basis sets, and effect of linearly dependent products of orbital basis functions. <i>Journal of Chemical Physics</i> , 2008, 128, 104104.	1.2	61
18	Density functionals for exchange and correlation energies: Exact conditions and comparison of approximations. <i>International Journal of Quantum Chemistry</i> , 1994, 49, 539-548.	1.0	60

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19	Exact high-density limit of correlation potential for two-electron density. <i>Journal of Chemical Physics</i> , 1999, 110, 10262-10268.	1.2	54
20	Approximate noninteracting kinetic energy functionals from a nonuniform scaling requirement. <i>International Journal of Quantum Chemistry</i> , 1991, 40, 379-388.	1.0	53
21	Time-independent density-functional theory for excited states of Coulomb systems. <i>Physical Review A</i> , 2012, 85, .	1.0	53
22	Direct first principles algorithm for the universal electron density functional. <i>Journal of Chemical Physics</i> , 1982, 77, 396-398.	1.2	52
23	Line-integral formulas for exchange and correlation potentials separately. <i>Physical Review A</i> , 1997, 55, 1885-1889.	1.0	47
24	A new functional with homogeneous coordinate scaling in density functional theory: $F_{\text{hom}}[\rho]$ . <i>Journal of Chemical Physics</i> , 1985, 83, 2334-2336.	1.2	46
25	Expectation values in density-functional theory, and kinetic contribution to the exchange-correlation energy. <i>Physical Review B</i> , 1993, 47, 1167-1173.	1.1	45
26	Time-independent (static) density-functional theories for pure excited states: Extensions and unification. <i>Physical Review A</i> , 2009, 80, .	1.0	44
27	Density-functional exchange identity from coordinate scaling. <i>Physical Review A</i> , 1996, 53, 3140-3142.	1.0	42
28	An energy-density equation for isoelectronic changes in atoms. <i>Journal of Chemical Physics</i> , 1978, 68, 5298-5299.	1.2	40
29	Sum rules for exchange and correlation potentials. <i>Journal of Chemical Physics</i> , 2001, 115, 4438-4443.	1.2	39
30	Ground-State Energy as a Simple Sum of Orbital Energies in Kohn-Sham Theory: A Shift in Perspective through a Shift in Potential. <i>Physical Review Letters</i> , 2014, 113, 113002.	2.9	39
31	Atomic binding energies from fundamental theorems involving the electron density, $\tilde{\rho}^{\text{hom}}$ , and the $Z^{\text{hom}}$ perturbation expansion. <i>Journal of Chemical Physics</i> , 1980, 72, 3416-3417.	1.2	37
32	Rigorous and approximate relations between expectation values of atoms. <i>Journal of Chemical Physics</i> , 1980, 72, 4009-4013.	1.2	37
33	Average Local Ionization Energies in the Hartree-Fock and Kohn-Sham Theories. <i>Journal of Physical Chemistry A</i> , 2009, 113, 1384-1389.	1.1	32
34	Success of quantum mechanical approximations for molecular geometries and electron-nuclear attraction expectation values: Gift of the Coulomb potential?. <i>Journal of Chemical Physics</i> , 1986, 84, 4519-4523.	1.2	30
35	Electron density-functional theory and x-ray structure factors. <i>Physical Review B</i> , 1987, 35, 7887-7890.	1.1	30
36	Recent constrained-search advances for approximating density functionals. <i>The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties</i> , 1994, 69, 763-769.	0.6	30

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37	A discontinuous energy-density functional. <i>Journal of Chemical Physics</i> , 1982, 77, 3140-3147.	1.2	28
38	Connections between ground-state energies from optimized-effective potential exchange-only and Hartree-Fock methods. <i>Journal of Chemical Physics</i> , 2003, 119, 7087-7093.	1.2	26
39	Method for direct determination of localized orbitals. <i>Journal of Chemical Physics</i> , 1975, 63, 316-318.	1.2	24
40	Accurate correlation potentials from integral formulation of density functional perturbation theory. <i>Journal of Chemical Physics</i> , 2002, 116, 6924-6929.	1.2	24
41	On approximate energy differences from average electron densities. <i>Journal of Chemical Physics</i> , 1979, 70, 1573-1574.	1.2	23
42	On the simple constrained-search reformulation of the Hohenberg-Kohn theorem to include degeneracies and more (1964-1979). <i>International Journal of Quantum Chemistry</i> , 2010, 110, 3140-3144.	1.0	23
43	Energy-density relations and screening constants in atoms. <i>Journal of Chemical Physics</i> , 1980, 73, 5168-5173.	1.2	22
44	Improving energies by using exact electron densities. <i>Physical Review A</i> , 1996, 53, R2915-R2917.	1.0	22
45	Augmented potential, energy densities, and virial relations in the weak- and strong-interaction limits of DFT. <i>Journal of Chemical Physics</i> , 2017, 147, 214107.	1.2	22
46	Connections between High-Density Scaling Limits of DFT Correlation Energies and Second-Order Z-1 Quantum Chemistry Correlation Energy. <i>Journal of Physical Chemistry A</i> , 1998, 102, 3151-3156.	1.1	20
47	Comment on "Functional derivative of the universal density functional in Fock space". <i>Physical Review A</i> , 2009, 79, .	1.0	17
48	Asymptotic coordinate scaling bound for exchange-correlation energy in density-functional theory. <i>International Journal of Quantum Chemistry</i> , 1989, 36, 617-619.	1.0	17
49	Bounds for the exchange and correlation potentials. <i>Physical Review A</i> , 1995, 51, 2851-2856.	1.0	15
50	Mathematical thoughts in DFT. <i>International Journal of Quantum Chemistry</i> , 2016, 116, 802-804.	1.0	12
51	Unconstrained exchange localization and distant orbital tails. <i>Journal of Chemical Physics</i> , 1976, 65, 2473-2475.	1.2	11
52	The nearest self-adjoint operator. <i>Journal of Chemical Physics</i> , 1980, 72, 780-781.	1.2	11
53	Kinetic energy from a single Kohn-Sham orbital. <i>Physical Review A</i> , 2009, 79, .	1.0	11
54	Energy differences from electrostatic potentials at nuclei. <i>Journal of Chemical Physics</i> , 1987, 87, 5044-5046.	1.2	10

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55	Approach to density-functional ionization energy. <i>Physical Review B</i> , 1996, 53, 969-972.	1.1	10
56	Formal expressions and corresponding expansions for the exact Kohn-Sham exchange potential. <i>Physical Review A</i> , 2009, 80, .	1.0	10
57	Kinetic and electron-electron energies for convex sums of ground state densities with degeneracies and fractional electron number. <i>Journal of Chemical Physics</i> , 2014, 140, 18A538.	1.2	10
58	Simple hydrogenic estimates for the exchange and correlation energies of atoms and atomic ions, with implications for density functional theory. <i>Journal of Chemical Physics</i> , 2020, 153, 074114.	1.2	10
59	Exact local exchange potential from Fock equations at vanishing coupling constant, and $\hat{T}_c/\hat{T}_n$ from wave-function calculations at full coupling constant. <i>Physical Review A</i> , 1996, 53, 3963-3965.	1.0	9
60	New exact relations for improving the exchange and correlation potentials. <i>International Journal of Quantum Chemistry</i> , 1995, 56, 385-388.	1.0	8
61	Closed-form expression relating the second-order component of the density functional theory correlation energy to its functional derivative. <i>Journal of Chemical Physics</i> , 1998, 109, 6280-6286.	1.2	8
62	Nodal variational principle for excited states. <i>Physical Review A</i> , 2018, 98, .	1.0	8
63	Highly Excited States from a Time Independent Density Functional Method. <i>Computation</i> , 2016, 4, 28.	1.0	7
64	Variational energy functionals involving one-electron operators. <i>Journal of Chemical Physics</i> , 1977, 67, 724-726.	1.2	6
65	Adiabatic integration formula for the correlation energy functional of the Hartree-Fock density. <i>Theoretical Chemistry Accounts</i> , 1999, 103, 117-123.	0.5	6
66	Tight constraints on the exchange-correlation potentials of degenerate states. <i>Journal of Chemical Physics</i> , 2014, 140, 18A537.	1.2	6
67	On augmented Kohn-Sham potential for energy as a simple sum of orbital energies. <i>Molecular Physics</i> , 2016, 114, 1162-1164.	0.8	6
68	Approximating the Shifted Hartree-Exchange-Correlation Potential in Direct Energy Kohn-Sham Theory. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 684-692.	2.3	6
69	Additive density functional correlation corrections to single particle theories. <i>International Journal of Quantum Chemistry</i> , 1997, 61, 281-285.	1.0	3
70	Properties of Augmented Kohn-Sham Potential for Energy as Simple Sum of Orbital Energies. <i>Journal of Physical Chemistry A</i> , 2017, 121, 342-347.	1.1	3
71	Density- and spin-density-functional theories through spin-free wave functions. <i>Physical Review A</i> , 2019, 100, .	1.0	3
72	On the best partitioning of the density functional energy. <i>Journal of Molecular Modeling</i> , 2018, 24, 311.	0.8	1

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73	THEOREMS FOR EXACT LOCAL EXCHANGE POTENTIAL. <i>Modern Physics Letters B</i> , 1991, 05, 1613-1616.	1.0	0
74	Pointwise and generalized virial theorems. <i>International Journal of Quantum Chemistry</i> , 1978, 14, 343-344.	1.0	0
75	Properties of the exact universal density and one-matrix functionals. <i>International Journal of Quantum Chemistry</i> , 1985, 28, 743-744.	1.0	0
76	Energy components in spin-density functional theory. <i>Physical Review A</i> , 2021, 104, .	1.0	0
77	Line-integral formulas for exchange and correlation potentials separately. <i>World Scientific Series in 20th Century Physics</i> , 2009, , 613-617.	0.0	0
78	On the adiabatic connection method, and scaling of electron-electron interactions in the Thomas-Fermi limit. <i>World Scientific Series in 20th Century Physics</i> , 2009, , 542-545.	0.0	0