Mel Levy

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/6296037/publications.pdf

Version: 2024-02-01

78 papers	13,402 citations	136950 32 h-index	79698 73 g-index
80 all docs	80 docs citations	80 times ranked	6591 citing authors

#	Article	IF	Citations
1	Energy components in spin-density functional theory. Physical Review A, 2021, 104, .	2.5	0
2	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.	3.0	10
3	Density- and spin-density-functional theories through spin-free wave functions. Physical Review A, 2019, 100, .	2.5	3
4	Approximating the Shifted Hartree-Exchange-Correlation Potential in Direct Energy Kohnâ€“Sham Theory. Journal of Chemical Theory and Computation, 2018, 14, 684-692.	5.3	6
5	On the best partitioning of the density functional energy. Journal of Molecular Modeling, 2018, 24, 311.	1.8	1
6	Nodal variational principle for excited states. Physical Review A, 2018, 98, .	2.5	8
7	Properties of Augmented Kohnâ€“Sham Potential for Energy as Simple Sum of Orbital Energies. Journal of Physical Chemistry A, 2017, 121, 342-347.	2.5	3
8	Augmented potential, energy densities, and virial relations in the weak- and strong-interaction limits of DFT. Journal of Chemical Physics, 2017, 147, 214107.	3.0	22
9	Highly Excited States from a Time Independent Density Functional Method. Computation, 2016, 4, 28.	2.0	7
10	Mathematical thoughts in DFT. International Journal of Quantum Chemistry, 2016, 116, 802-804.	2.0	12
11	On augmented Kohnâ€“Sham potential for energy as a simple sum of orbital energies. Molecular Physics, 2016, 114, 1162-1164.	1.7	6
12	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.	3.0	10
13	Tight constraints on the exchange-correlation potentials of degenerate states. Journal of Chemical Physics, 2014, 140, 18A537.	3.0	6
14	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.	7.8	39
15	Time-independent density-functional theory for excited states of Coulomb systems. Physical Review A, 2012, 85, .	2.5	53
16	On the simple constrainedâ€search reformulation of the Hohenbergâ€“Kohn theorem to include degeneracies and more (1964â€“1979). International Journal of Quantum Chemistry, 2010, 110, 3140-3144.	2.0	23
17	Comment on â€œFunctional derivative of the universal density functional in Fock spaceâ€• Physical Review A, 2009, 79, .	2.5	17
18	Kinetic energy from a single Kohn-Sham orbital. Physical Review A, 2009, 79, .	2.5	11

#	Article	IF	Citations
19	Average Local Ionization Energies in the Hartreeâ^'Fock and Kohnâ^'Sham Theories. Journal of Physical Chemistry A, 2009, 113, 1384-1389.	2.5	32
20	Time-independent (static) density-functional theories for pure excited states: Extensions and unification. Physical Review A, 2009, 80, .	2.5	44
21	Formal expressions and corresponding expansions for the exact Kohn-Sham exchange potential. Physical Review A, 2009, 80, .	2.5	10
22	Line-integral formulas for exchange and correlation potentials separately. World Scientific Series in 20th Century Physics, 2009, , 613-617.	0.0	0
23	On the adiabatic connection method, and scaling of electronâ€"electron interactions in the Thomasâ€"Fermi limit. World Scientific Series in 20th Century Physics, 2009, , 542-545.	0.0	0
24	Relation between exchange-only optimized potential and Kohnâ€"Sham methods with finite basis sets, and effect of linearly dependent products of orbital basis functions. Journal of Chemical Physics, 2008, 128, 104104.	3.0	61
25	Generalized density-functional theory: Conquering theN-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.	1.5	79
26	Connections between ground-state energies from optimized-effective potential exchange-only and Hartreeâ€"Fock methods. Journal of Chemical Physics, 2003, 119, 7087-7093.	3.0	26
27	Accurate correlation potentials from integral formulation of density functional perturbation theory. Journal of Chemical Physics, 2002, 116, 6924-6929.	3.0	24
28	Sum rules for exchange and correlation potentials. Journal of Chemical Physics, 2001, 115, 4438-4443.	3.0	39
29	Perspective on "Density functional approach to the frontier-electron theory of chemical reactivity". Theoretical Chemistry Accounts, 2000, 103, 353-360.	1.4	424
30	Strictly correlated electrons in density-functional theory. Physical Review A, 1999, 59, 51-54.	2.5	146
31	Exact high-density limit of correlation potential for two-electron density. Journal of Chemical Physics, 1999, 110, 10262-10268.	3.0	54
32	Adiabatic integration formula for the correlation energy functional of the Hartree-Fock density. Theoretical Chemistry Accounts, 1999, 103, 117-123.	1.4	6
33	Variational Density-Functional Theory for an Individual Excited State. Physical Review Letters, 1999, 83, 4361-4364.	7.8	180
34	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.	3.0	8
35	Connections between High-Density Scaling Limits of DFT Correlation Energies and Second-OrderZ-1Quantum Chemistry Correlation Energy. Journal of Physical Chemistry A, 1998, 102, 3151-3156.	2.5	20
36	Line-integral formulas for exchange and correlation potentials separately. Physical Review A, 1997, 55, 1885-1889.	2.5	47

#	Article	IF	Citations
37	Hybrid schemes combining the Hartreeâ€“Fock method and density-functional theory: Underlying formalism and properties of correlation functionals. Journal of Chemical Physics, 1997, 106, 2675-2680.	3.0	97
38	Additive density functional correlation corrections to single particle theories. International Journal of Quantum Chemistry, 1997, 61, 281-285.	2.0	3
39	Approach to density-functional ionization energy. Physical Review B, 1996, 53, 969-972.	3.2	10
40	Exact local exchange potential from Fock equations at vanishing coupling constant, and ÎTc/Î´from wave-function calculations at full coupling constant. Physical Review A, 1996, 53, 3963-3965.	2.5	9
41	Density-functional exchange identity from coordinate scaling. Physical Review A, 1996, 53, 3140-3142.	2.5	42
42	Improving energies by using exact electron densities. Physical Review A, 1996, 53, R2915-R2917.	2.5	22
43	New exact relations for improving the exchange and correlation potentials. International Journal of Quantum Chemistry, 1995, 56, 385-388.	2.0	8
44	DFT ionization formulas and aDFT perturbation theory for exchange and correlation, through adiabatic connection. International Journal of Quantum Chemistry, 1995, 56, 93-108.	2.0	142
45	Correlation-energy density-functional formulas from correlating first-order density matrices. Physical Review A, 1995, 52, R1808-R1810.	2.5	98
46	Bounds for the exchange and correlation potentials. Physical Review A, 1995, 51, 2851-2856.	2.5	15
47	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.	0.6	30
48	Exact Kohn-Sham scheme based on perturbation theory. Physical Review A, 1994, 50, 196-204.	2.5	506
49	Density functionals for exchange and correlation energies: Exact conditions and comparison of approximations. International Journal of Quantum Chemistry, 1994, 49, 539-548.	2.0	60
50	Correlation-energy functional and its high-density limit obtained from a coupling-constant perturbation expansion. Physical Review B, 1993, 47, 13105-13113.	3.2	385
51	Expectation values in density-functional theory, and kinetic contribution to the exchange-correlation energy. Physical Review B, 1993, 47, 1167-1173.	3.2	45
52	Approximate noninteracting kinetic energy functionals from a nonuniform scaling requirement. International Journal of Quantum Chemistry, 1991, 40, 379-388.	2.0	53
53	Density-functional exchange correlation through coordinate scaling in adiabatic connection and correlation hole. Physical Review A, 1991, 43, 4637-4646.	2.5	261
54	THEOREMS FOR EXACT LOCAL EXCHANGE POTENTIAL. Modern Physics Letters B, 1991, 05, 1613-1616.	1.9	0

#	Article	IF	Citations
55	Asymptotic coordinate scaling bound for exchange-correlation energy in density-functional theory. International Journal of Quantum Chemistry, 1989, 36, 617-619.	2.0	17
56	Electron density-functional theory and x-ray structure factors. Physical Review B, 1987, 35, 7887-7890.	3.2	30
57	Energy differences from electrostatic potentials at nuclei. Journal of Chemical Physics, 1987, 87, 5044-5046.	3.0	10
58	Success of quantum mechanical approximations for molecular geometries and electronâ€“nuclear attraction expectation values: Gift of the Coulomb potential?. Journal of Chemical Physics, 1986, 84, 4519-4523.	3.0	30
59	A new functional with homogeneous coordinate scaling in density functional theory: Fâ€‰[â€‰ï¸Î»]. Journal of Chemical Physics, 1985, 83, 2334-2336.	3.0	46
60	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.	2.5	897
61	Properties of the exact universal density and one-matrix functionals. International Journal of Quantum Chemistry, 1985, 28, 743-744.	2.0	0
62	Exact differential equation for the density and ionization energy of a many-particle system. Physical Review A, 1984, 30, 2745-2748.	2.5	803
63	Physical Content of the Exact Kohn-Sham Orbital Energies: Band Gaps and Derivative Discontinuities. Physical Review Letters, 1983, 51, 1884-1887.	7.8	2,105
64	Direct first principles algorithm for the universal electron density functional. Journal of Chemical Physics, 1982, 77, 396-398.	3.0	52
65	A discontinuous energyâ€“density functional. Journal of Chemical Physics, 1982, 77, 3140-3147.	3.0	28
66	Electron densities in search of Hamiltonians. Physical Review A, 1982, 26, 1200-1208.	2.5	570
67	Density-Functional Theory for Fractional Particle Number: Derivative Discontinuities of the Energy. Physical Review Letters, 1982, 49, 1691-1694.	7.8	2,573
68	Energyâ€density relations and screening constants in atoms. Journal of Chemical Physics, 1980, 73, 5168-5173.	3.0	22
69	Atomic binding energies from fundamental theorems involving the electron density, ã€ˆrâˆ’1ã€‰, and the Zâˆ’1 perturbation expansion. Journal of Chemical Physics, 1980, 72, 3416-3417.	3.0	37
70	The nearest selfâ€adjoint operator. Journal of Chemical Physics, 1980, 72, 780-781.	3.0	11
71	Rigorous and approximate relations between expectation values of atoms. Journal of Chemical Physics, 1980, 72, 4009-4013.	3.0	37
72	On approximate energy differences from average electron densities. Journal of Chemical Physics, 1979, 70, 1573-1574.	3.0	23

#	Article	IF	Citations
73	Electronegativity: The density functional viewpoint. Journal of Chemical Physics, 1978, 68, 3801-3807.	3.0	2,806
74	An energyâ€density equation for isoelectronic changes in atoms. Journal of Chemical Physics, 1978, 68, 5298-5299.	3.0	40
75	Pointwise and generalized virial theorems. International Journal of Quantum Chemistry, 1978, 14, 343-344.	2.0	0
76	Variational energy functionals involving oneâ€electron operators. Journal of Chemical Physics, 1977, 67, 724-726.	3.0	6
77	Unconstrained exchange localization and distant orbital tails. Journal of Chemical Physics, 1976, 65, 2473-2475.	3.0	11
78	Method for direct determination of localized orbitals. Journal of Chemical Physics, 1975, 63, 316-318.	3.0	24