Agnes Nagy

List of Publications by Year
in descending order

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161 papers	3,416 citations	126907 33 h-index	182427 51 g-index
161 all docs	161 docs citations	161 times ranked	918 citing authors

#	Article	IF	Citations
1	Variational Density-Functional Theory for an Individual Excited State. Physical Review Letters, 1999, 83, 4361-4364.	7.8	180
2	Density functional. Theory and application to atoms and molecules. Physics Reports, 1998, 298, 1-79.	25.6	151
3	Local kinetic energy and local temperature in the density-functional theory of electronic structure. International Journal of Quantum Chemistry, 2002, 90, 309-326.	2.0	139
4	Fisher information in density functional theory. Journal of Chemical Physics, 2003, 119, 9401-9405.	3.0	104
5	Variational density-functional theory for degenerate excited states. Physical Review A, 2001, 63, .	2.5	82
6	Fisher information in a two-electron entangled artificial atom. Chemical Physics Letters, 2006, 425, 154-156.	2.6	76
7	Density-matrix functional theory. Physical Review A, 2002, 66, .	2.5	69
8	Fisher information and steric effect. Chemical Physics Letters, 2007, 449, 212-215.	2.6	69
9	Excited states in density functional theory. International Journal of Quantum Chemistry, 1998, 70, 681-691.	2.0	63
10	Local wave-vector, Shannon and Fisher information. Physics Letters, Section A: General, Atomic and Solid State Physics, 2008, 372, 1654-1656.	2.1	59
11	Parameter-free exchange potential for excitation in the density-functional theory: Application to excitation energies within the fractional-occupation approach. Physical Review A, 1990, 42, 4388-4390.	2.5	54
12	Effective potential in density matrix functional theory. Journal of Chemical Physics, 2004, 121, 6640-6648.	3.0	54
13	Time-independent density-functional theory for excited states of Coulomb systems. Physical Review A, 2012, 85, .	2.5	53
14	Kohn-Sham equations for multiplets. Physical Review A, 1998, 57, 1672-1677.	2.5	51
15	A generalized statistical complexity measure: Applications to quantum systems. Journal of Mathematical Physics, 2009, 50, .	1.1	51
16	The Fisherâ€“Shannon information plane for atoms. Physics Letters, Section A: General, Atomic and Solid State Physics, 2008, 372, 2428-2430.	2.1	49
17	Ground- and excited-state cusp conditions for the electron density. Journal of Chemical Physics, 2001, 115, 6300-6308.	3.0	48
18	Fisherâ€“RÃ©nyi entropy product and information plane. Physics Letters, Section A: General, Atomic and Solid State Physics, 2008, 372, 6823-6825.	2.1	47

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19	RÃ©nyi information of atoms. Physics Letters, Section A: General, Atomic and Solid State Physics, 2008, 372, 4918-4922.	2.1	46
20	Fisher and Shannon information in orbitalâ€free density functional theory. International Journal of Quantum Chemistry, 2015, 115, 1392-1395.	2.0	45
21	Local ensemble exchange potential. Journal of Physics B: Atomic, Molecular and Optical Physics, 1996, 29, 389-394.	1.5	44
22	Alternative derivation of the Krieger-Li-Iafrate approximation to the optimized-effective-potential method. Physical Review A, 1997, 55, 3465-3468.	2.5	44
23	Shannon entropy density as a descriptor of Coulomb systems. Chemical Physics Letters, 2013, 556, 355-358.	2.6	44
24	Atomic Fisher information versus atomic number. Physics Letters, Section A: General, Atomic and Solid State Physics, 2006, 360, 291-293.	2.1	43
25	Relativistic density-functional theory for ensembles of excited states. Physical Review A, 1994, 49, 3074-3076.	2.5	42
26	Exchange energy in the exact exchange-only density functional theory. Journal of Physics B: Atomic, Molecular and Optical Physics, 1993, 26, 43-48.	1.5	41
27	Coordinate scaling and adiabatic connection formula for ensembles of fractionally occupied excited states. International Journal of Quantum Chemistry, 1995, 56, 225-228.	2.0	41
28	Higher-order cusp of the density in certain highly excited states of atoms and molecules. Journal of Physics B: Atomic, Molecular and Optical Physics, 2000, 33, 1745-1751.	1.5	41
29	Information entropy as a measure of the quality of an approximate electronic wave function. International Journal of Quantum Chemistry, 1998, 58, 323-327.	2.0	36
30	Signatures of quantum fluctuations in the Dicke model by means of RÃ©nyi uncertainty. Physical Review A, 2012, 85, .	2.5	35
31	Optimized potential method for ensembles of excited states. International Journal of Quantum Chemistry, 1998, 69, 247-254.	2.0	34
32	The Pauli potential from the differential virial theorem. International Journal of Quantum Chemistry, 2010, 110, 2117-2120.	2.0	34
33	Excitation energies calculated with parameter-free exchange potential in the density functional theory. Journal of Physics B: Atomic, Molecular and Optical Physics, 1991, 24, 4691-4694.	1.5	33
34	Communication: Kohn-Sham theory for excited states of Coulomb systems. Journal of Chemical Physics, 2015, 143, 191101.	3.0	33
35	Exact potential-phase relation for the ground state of the C atom. Physical Review A, 1989, 40, 554-557.	2.5	32
36	Exact ensemble exchange potentials for multiplets. International Journal of Quantum Chemistry, 1995, 56, 297-301.	2.0	32

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37	Maximum RÃ©nyi entropy principle and the generalized Thomasâ€“Fermi model. Physics Letters, Section A: General, Atomic and Solid State Physics, 2009, 373, 844-846.	2.1	32
38	Alternatives to the electron density for describing Coulomb systems. Journal of Chemical Physics, 2007, 126, 144108.	3.0	31
39	RÃ©nyi entropy and quantum phase transition in the Dicke model. Physics Letters, Section A: General, Atomic and Solid State Physics, 2011, 375, 3066-3069.	2.1	31
40	Excitation energies in the local density functional theory. Journal of Physics B: Atomic, Molecular and Optical Physics, 1994, 27, 233-240.	1.5	30
41	Phase-space Fisher information. Chemical Physics Letters, 2007, 437, 132-137.	2.6	30
42	Relative RÃ©nyi entropy for atoms. International Journal of Quantum Chemistry, 2009, 109, 2490-2494.	2.0	30
43	Relative RÃ©nyi entropy and fidelity susceptibility. Europhysics Letters, 2015, 109, 60002.	2.0	30
44	An alternative optimized potential method for ensembles of excited states. Journal of Physics B: Atomic, Molecular and Optical Physics, 2001, 34, 2363-2370.	1.5	29
45	Hierarchy of equations in the generalized density functional theory. International Journal of Quantum Chemistry, 2006, 106, 1043-1051.	2.0	29
46	Excitation energies in density functional theory: comparison of several methods for the H2O, N2, CO and C2H4 molecules. Chemical Physics Letters, 1998, 296, 489-493.	2.6	28
47	Exact results on the curvature of the electron density at the cusp in certain highly excited states of atoms. Chemical Physics Letters, 2000, 332, 154-158.	2.6	28
48	Generalized density functional theory for degenerate states. Journal of Chemical Physics, 2005, 122, 134107.	3.0	28
49	LMC complexity for the ground states of different quantum systems. Physics Letters, Section A: General, Atomic and Solid State Physics, 2009, 373, 2552-2555.	2.1	28
50	Analysis of the Pauli potential of atoms and ions. Acta Physica Hungarica, 1991, 70, 321-331.	0.1	27
51	Ratio of density gradient to electron density as a local wavenumber to characterize the ground state of spherical atoms. Molecular Physics, 1997, 90, 271-276.	1.7	27
52	Functional derivative of the kinetic energy functional for spherically symmetric systems. Journal of Chemical Physics, 2011, 135, 044106.	3.0	27
53	Fisher information, RÃ©nyi entropy power and quantum phase transition in the Dicke model. Physica A: Statistical Mechanics and Its Applications, 2012, 391, 3650-3655.	2.6	27
54	Density functional theory for excited states. Advances in Quantum Chemistry, 1998, , 159-178.	0.8	26

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55	Exact and approximate exchange potentials in the density functional theory. The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties, 1994, 69, 779-785.	0.6	25
56	Density functional theory as thermodynamics. Journal of Chemical Sciences, 1994, 106, 217-227.	1.5	25
57	Spherically and system-averaged pair density functional theory. Journal of Chemical Physics, 2006, 125, 184104.	3.0	23
58	Alternative descriptors of Coulomb systems and their relationship to the kinetic energy. Chemical Physics Letters, 2008, 460, 343-346.	2.6	22
59	A generalized relative complexity measure. Journal of Statistical Mechanics: Theory and Experiment, 2011, 2011, P09016.	2.3	22
60	Time-independent density functional theory for degenerate excited states of Coulomb systems. Theoretical Chemistry Accounts, 2018, 137, 1.	1.4	22
61	Density Functional Theory description of the order-disorder transformation in Fe-Ni. Scientific Reports, 2019, 9, 8172.	3.3	22
62	Conceptual Problem with Calculating Electron Densities in Finite Basis Density Functional Theory. Journal of Chemical Theory and Computation, 2017, 13, 3961-3963.	5.3	21
63	Hardness and excitation energy. Journal of Chemical Sciences, 2005, 117, 437-440.	1.5	20
64	Relation between Fisher measures of information coming from pair distribution functions. Chemical Physics Letters, 2010, 490, 242-244.	2.6	19
65	Differential equation for ground-state electron density of He-like ions for large atomic number. Chemical Physics Letters, 1999, 305, 429-432.	2.6	18
66	Remarks on density functional theory as a thermodynamics. Computational and Theoretical Chemistry, 2000, 501-502, 101-106.	1.5	17
67	Density scaling and exchange-correlation energy. Journal of Chemical Physics, 2005, 123, 044105.	3.0	15
68	RÃ©nyiâ€“Fisher entropy product as a marker of topological phase transitions. Physica A: Statistical Mechanics and Its Applications, 2018, 498, 66-73.	2.6	15
69	Electron-electron cusp condition and asymptotic behavior for the Pauli potential in pair density functional theory. Journal of Chemical Physics, 2008, 128, 114115.	3.0	14
70	Binding Entropy and Its Application to Solids. Journal of Physical Chemistry A, 2009, 113, 9022-9029.	2.5	14
71	Local coordinate, wave vector, Fisher and Shannon information in momentum representation. Physics Letters, Section A: General, Atomic and Solid State Physics, 2013, 377, 286-290.	2.1	14
72	Relative information in excitedâ€state orbitalâ€free density functional theory. International Journal of Quantum Chemistry, 2020, 120, e26405.	2.0	14

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73	Ghost- and self-interaction-free ensemble calculations with local exchangeâ€“correlation potential for atoms. Journal of Physics B: Atomic, Molecular and Optical Physics, 2003, 36, 4073-4080.	1.5	13
74	Fisher and Shannon information from one-matrix. Link to the kinetic energy. Chemical Physics Letters, 2014, 597, 139-142.	2.6	13
75	Density functional theory from spherically symmetric densities. Journal of Chemical Physics, 2018, 149, 204112.	3.0	13
76	A method to get an analytical expression for the non-interacting kinetic energy density functional. Computational and Theoretical Chemistry, 2000, 501-502, 167-171.	1.5	12
77	An approximation to the ensemble Kohnâ€“Sham exchange potential for excited states of atoms. Journal of Chemical Physics, 2003, 119, 4141-4147.	3.0	12
78	A Density Functional Theory View of Quantum Phase Transitions. Journal of Chemical Theory and Computation, 2013, 9, 1068-1072.	5.3	12
79	Cusp relation for the Pauli potential. Physical Review A, 2014, 90, .	2.5	12
80	Exchange-Correlation Catastrophe in Cu-Au: A Challenge for Semilocal Density Functional Approximations. Physical Review Letters, 2016, 117, 066401.	7.8	12
81	Thermodynamical transcription of the density functional theory with constant temperature. International Journal of Quantum Chemistry, 2017, 117, e25396.	2.0	12
82	Theories for excited states. Advances in Quantum Chemistry, 2003, 42, 363-381.	0.8	11
83	Alternative to the Kohn-Sham equations: The Pauli potential differential equation. Physical Review A, 2015, 92, .	2.5	11
84	Thermodynamical transcription of density functional theory with minimum Fisher information. Chemical Physics Letters, 2018, 695, 149-152.	2.6	11
85	Inequalities for phaseâ€space RÃ©nyi entropies. International Journal of Quantum Chemistry, 2012, 112, 1285-1290.	2.0	10
86	Ground- and excited-state cusp conditions for the pair density. Physical Review A, 2010, 82, .	2.5	9
87	RÃ©nyi entropy of the U(3) vibron model. Journal of Mathematical Chemistry, 2013, 51, 620-636.	1.5	9
88	Density functional fidelity susceptibility and Kullbackâ€“Leibler entropy. Physics Letters, Section A: General, Atomic and Solid State Physics, 2013, 377, 3098-3101.	2.1	9
89	Fisher information and RÃ©nyi dimensions: A thermodynamical formalism. Chaos, 2016, 26, 083102.	2.5	9
90	Pair Density Functional Theory. Progress in Theoretical Chemistry and Physics, 2003, , 79-87.	0.2	9

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91	Total electron density from thes-electron density. Physical Review A, 1998, 57, 3458-3461.	2.5	8
92	A generalized Kohnâ€“Sham scheme. Chemical Physics Letters, 2005, 411, 492-495.	2.6	8
93	Differential virial theorem in density-functional theory in terms of the Pauli potential for spherically symmetric electron densities: Illustrative example for the family of Be-like atomic ions. Physical Review A, 2008, 78, .	2.5	8
94	Quantum phase transitions via density-functional theory: Extension to the degenerate case. Physical Review A, 2013, 88, .	2.5	8
95	Theories for individual excited states. International Journal of Quantum Chemistry, 2004, 99, 256-264.	2.0	7
96	Time-dependent density functional theory as a thermodynamics. Computational and Theoretical Chemistry, 2010, 943, 48-52.	1.5	7
97	Generalized complexity measures and chaotic maps. Chaos, 2012, 22, 023118.	2.5	7
98	Fisher information and RÃ©nyi entropies in dynamical systems. Chaos, 2017, 27, 073104.	2.5	7
99	Fisher information and density functional theory. International Journal of Quantum Chemistry, 2022, 122, e26679.	2.0	7
100	Determination of the total electron density from its l -shell contribution. Computational and Theoretical Chemistry, 2000, 501-502, 107-113.	1.5	6
101	DENSITY FUNCTIONAL THEORY AS THERMODYNAMICS. , 2002, , 413-443.		6
102	Study of subspace density functional theory application of LSDA to excited states of atoms. International Journal of Quantum Chemistry, 2003, 92, 234-238.	2.0	6
103	Approximate ansatz for the expansion of the spherically averaged wave function in terms of interelectronic separation r12 for the Hookean atom, atomic ions, and the H2 molecule. International Journal of Quantum Chemistry, 2003, 95, 21-29.	2.0	6
104	Excited-state pair-density-functional theory. Physical Review A, 2014, 90, .	2.5	6
105	<scp>K</scp>ullbackâ€“<scp>L</scp>eibler and relative <scp>F</scp>isher information as descriptors of locality. International Journal of Quantum Chemistry, 2018, 118, e25557.	2.0	6
106	Fidelity as a marker of topological phase transitions in 2D Dirac materials. International Journal of Quantum Chemistry, 2018, 118, e25674.	2.0	6
107	Integral and regional virial theorems in density functional theory. Journal of Chemical Sciences, 1994, 106, 251-258.	1.5	6
108	Total energy versus one-electron energy differences in the excited-state density functional theory. Journal of Physics B: Atomic, Molecular and Optical Physics, 2000, 33, L585-L589.	1.5	5

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109	Local self-interaction-free approximate exchange-correlation potentials in the variational density functional theory for individual excited states. Chemical Physics Letters, 2002, 366, 496-503.	2.6	5
110	Subspace density of the first excited state for two harmonically interacting electrons with isotropic harmonic confinement. Physics Letters, Section A: General, Atomic and Solid State Physics, 2005, 335, 347-350.	2.1	5
111	Exact differential and integral constraints for the Pauli potential in the pair density functional theory. Chemical Physics Letters, 2009, 469, 353-356.	2.6	5
112	A thermal orbital-free density functional approach. Journal of Chemical Physics, 2019, 151, 014103.	3.0	5
113	Density functional theory description of random Cu-Au alloys. Physical Review B, 2019, 99, .	3.2	5
114	Spherical Density Functional Theory and Atoms in Molecules. Journal of Physical Chemistry A, 2020, 124, 148-151.	2.5	5
115	Information theoretical and thermodynamic view of the excited-state density functional theory of Coulomb systems. Journal of Chemical Physics, 2020, 153, 154103.	3.0	5
116	Density Functional Theory for A Single Excited State. , 1999, , 451-462.		5
117	Spherical potential functional theory. Journal of Chemical Physics, 2021, 155, 144108.	3.0	5
118	Exchange-Only Theory: Relation Between Exchange Energy, Its Functional Derivative and Eigenvalue Sums in an Inhomogeneous Electron Liquid. Physics and Chemistry of Liquids, 1999, 37, 671-676.	1.2	4
119	Ten-Electron Central Field Problem: An Inhomogeneous Electron Liquid. Physics and Chemistry of Liquids, 2002, 40, 47-56.	1.2	4
120	Non-relativistic binding energies of heavy neutral atoms: Dependence of correlation energy on atomic number. Chemical Physics Letters, 2005, 416, 104-106.	2.6	4
121	Density scaling and relaxation of the Pauli principle. Journal of Chemical Physics, 2007, 126, 124111.	3.0	4
122	Modeling the Pauli potential in the pair density functional theory. Journal of Chemical Physics, 2008, 129, 204108.	3.0	4
123	Pauli potential in terms of kinetic energy density and electron density in the leading Coulombic term of the nonrelativistic1/Zexpansion of spherical atomic ions. Physical Review A, 2010, 81, .	2.5	4
124	Density and pair-density scaling for deriving the Euler equation in density-functional and pair-density-functional theory. Physical Review A, 2011, 84, .	2.5	4
125	Link between generalized nonidempotency and complexity measures. Journal of Molecular Modeling, 2017, 23, 159.	1.8	4
126	Time-dependent pair density functional theory. European Physical Journal B, 2018, 91, 1.	1.5	4

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127	Subspace theory with spherically symmetric densities. Journal of Chemical Physics, 2021, 154, 074103.	3.0	4
128	Exact integral relation between the triplet correlation function in the ground state of the completely polarised homogeneous electron fluid and the pair function: comparison with the classical liquid argon result. Physics and Chemistry of Liquids, 2009, 47, 5-8.	1.2	3
129	Pauli potential functional for spherical inhomogeneous electron liquids generated by a bare Coulomb field. Physics and Chemistry of Liquids, 2012, 50, 412-414.	1.2	3
130	Some model inhomogeneous electron liquid inDdimensions: relation between energy and chemical potential and a spatial generalisation of Kato's nuclear cusp theorem. Physics and Chemistry of Liquids, 2012, 50, 266-270.	1.2	3
131	Complexity measure and quantum shape-phase transitions in the two-dimensional limit of the vibron model. Journal of Molecular Modeling, 2014, 20, 2237.	1.8	3
132	Detecting regular and chaotic behaviour in the parameter space by generalised statistical complexity measures. Chaos, Solitons and Fractals, 2015, 78, 26-32.	5.1	3
133	Phase-space Fisher information of 2D gapped Dirac materials. Journal of Mathematical Chemistry, 2019, 57, 1169-1180.	1.5	3
134	Phase Space View of Ensembles of Excited States. Wuli Huaxue Xuebao/ Acta Physico - Chimica Sinica, 2018, 34, 492-496.	4.9	3
135	Theory of the Inhomogeneous Electron Liquid, Transcending Hartree-Fock. Physics and Chemistry of Liquids, 1992, 24, 183-191.	1.2	2
136	Exact expressions for energy functional in the time-dependent density functional theory. International Journal of Quantum Chemistry, 2003, 92, 229-233.	2.0	2
137	Exact energy expression in the strong-interaction limit of the density functional theory. Philosophical Magazine, 2006, 86, 2101-2114.	1.6	2
138	RÃ©nyi Entropy and Complexity. , 2011, , 215-235.		2
139	Density scaling for multiplets. Journal of Physics B: Atomic, Molecular and Optical Physics, 2011, 44, 035001.	1.5	2
140	Euler equation for descriptors of the spherically symmetric coulomb systems. International Journal of Quantum Chemistry, 2016, 116, 862-866.	2.0	2
141	Time-dependent pair density from the principle of minimum Fisher information. Journal of Molecular Modeling, 2018, 24, 234.	1.8	2
142	Coordinate Scaling in Time-Independent Excited-State Density Functional Theory for Coulomb Systems. Computation, 2019, 7, 59.	2.0	2
143	Density Functional Theory of Highly Excited States of Coulomb Systems. Computation, 2021, 9, 73.	2.0	2
144	Density Functional Theory of Coulombic Excited States Based on Nodal Variational Principle. Computation, 2021, 9, 93.	2.0	2

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145	Phase-space RÃ©nyi entropy, complexity and thermodynamic picture of density functional theory. Journal of Mathematical Chemistry, 2023, 61, 296-304.	1.5	2
146	Kinetic and exchange energy related non-locally in Hartreeâ€“Fock theory of an inhomogeneous electron liquid. Physics and Chemistry of Liquids, 2006, 44, 493-499.	1.2	1
147	Scaling of some chemical properties of tetrahedral and octahedral molecules plus almost spherical C and B cages. Journal of Mathematical Chemistry, 2011, 49, 2268-2274.	1.5	1
148	Relationship between the effective potentials determining the density and the pair density. Computational and Theoretical Chemistry, 2013, 1003, 97-100.	2.5	1
149	Kinetic Energy and Fisher Information. Recent Advances in Computational, 2013, , 387-400.	0.8	1
150	Theory of Excited States of Finite Systems in Coulomb External Potential. Journal of Physics: Conference Series, 2013, 410, 012155.	0.4	1
151	Density scaling and virial theorem. Molecular Physics, 2015, 113, 1839-1842.	1.7	1
152	Special Issue â€œ50th Anniversary of the Kohnâ€“Sham Theoryâ€”Advances in Density Functional Theoryâ€. Computation, 2016, 4, 45.	2.0	1
153	Orbital-Free Density Functional Theory: Pauli Potential and Density Scaling. , 2018, , 253-260.		1
154	Density Scaling for Excited States. Progress in Theoretical Chemistry and Physics, 2012, , 185-197.	0.2	1
155	Time-Independent Theories for a Single Excited State. , 2009, , .		1
156	Effective potential of a single excited state along the adiabatic path. Advances in Quantum Chemistry, 2001, 39, 35-46.	0.8	0
157	THEORY FOR A SINGLE EXCITED STATE DIFFERENTIAL VIRIAL THEOREM. Recent Advances in Computational, 2002, , 247-256.	0.8	0
158	Asymptotic form at large<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi mathvariant="bold-italic">r</mml:mi></mml:math>of a third-order linear homogeneous differential equation for the ground-state electron density of the He atom. Physical Review A, 2008, 77, .	2.5	0
159	Proposed approximate relation in inhomogeneous electron liquids between exchange-only potential and its Slater counterpart. Physics and Chemistry of Liquids, 2010, 48, 648-651.	1.2	0
160	Fisher information and topological pressure. Journal of Mathematical Physics, 2017, 58, 052702.	1.1	0
161	Formally exact integral equation theory of the exchange-only potential in density functional theory: Refined closure approximation. World Scientific Series in 20th Century Physics, 2009, , 720-724.	0.0	0