Andreas Savin

List of Publications by Year
in descending order

131 papers	17,352 citations	41344 49 h-index	14759 127 g-index
135 all docs	135 docs citations	135 times ranked	11669 citing authors

#	Article	IF	Citations
1	Results obtained with the correlation energy density functionals of becke and Lee, Yang and Parr. Chemical Physics Letters, 1989, 157, 200-206.	2.6	6,521
2	ELF: The Electron Localization Function. Angewandte Chemie International Edition in English, 1997, 36, 1808-1832.	4.4	1,929
3	Electron Localization in Solid-State Structures of the Elements: the Diamond Structure. Angewandte Chemie International Edition in English, 1992, 31, 187-188.	4.4	912
4	Combining long-range configuration interaction with short-range density functionals. Chemical Physics Letters, 1997, 275, 151-160.	2.6	681
5	Long-rangeâ€“short-range separation of the electron-electron interaction in density-functional theory. Physical Review A, 2004, 70, .	2.5	381
6	Escaping the symmetry dilemma through a pair-density interpretation of spin-density functional theory. Physical Review A, 1995, 51, 4531-4541.	2.5	335
7	van der Waals forces in density functional theory: Perturbational long-range electron-interaction corrections. Physical Review A, 2005, 72, .	2.5	287
8	Density functionals for the Yukawa electron-electron interaction. International Journal of Quantum Chemistry, 1995, 56, 327-332.	2.0	261
9	Adiabatic-Connection Fluctuation-Dissipation Density-Functional Theory Based on Range Separation. Physical Review Letters, 2009, 102, 096404.	7.8	240
10	A Systematic Failing of Current Density Functionals:â€‰ Overestimation of Two-Center Three-Electron Bonding Energies. Journal of Physical Chemistry A, 1998, 102, 7872-7877.	2.5	234
11	Die Elektronenlokalisierungsfunktion ELF. Angewandte Chemie, 1997, 109, 1892-1918.	2.0	190
12	Double-hybrid density-functional theory made rigorous. Journal of Chemical Physics, 2011, 134, 064113.	3.0	165
13	Assessment of a Middle-Range Hybrid Functional. Journal of Chemical Theory and Computation, 2008, 4, 1254-1262.	5.3	155
14	The importance of middle-range Hartree-Fock-type exchange for hybrid density functionals. Journal of Chemical Physics, 2007, 127, 221103.	3.0	152
15	A correlation-energy density functional for multideterminantal wavefunctions. Molecular Physics, 1997, 91, 527-536.	1.7	149
16	The electron localization function (ELF) and its relatives: interpretations and difficulties. Computational and Theoretical Chemistry, 2005, 727, 127-131.	1.5	144
17	Virtual space level shifting and correlation energies. International Journal of Quantum Chemistry, 1998, 69, 581-590.	2.0	143
18	On the Bonding in Carbosilanes. Angewandte Chemie International Edition in English, 1992, 31, 185-187.	4.4	137

#	Article	IF	Citations
19	Hybrid functionals with local range separation. Journal of Chemical Physics, 2008, 129, 124103.	3.0	134
20	A short-range gradient-corrected spin density functional in combination with long-range coupled-cluster methods: Application to alkali-metal rare-gas dimers. Chemical Physics, 2006, 329, 276-282.	1.9	133
21	Strictly correlated electrons in density-functional theory: A general formulation with applications to spherical densities. Physical Review A, 2007, 75, .	2.5	126
22	Construction of An Accurate Self-interaction-corrected Correlation Energy Functional Based on An Electron Gas with A Gap. , 1999, , 463-477.		122
23	Die Elektronenlokalisierung in den FestkÃ¶rperâ€strukturen der Elemente: die Diamantstruktur. Angewandte Chemie, 1992, 104, 186-188.	2.0	121
24	Short-range exchange and correlation energy density functionals: Beyond the local-density approximation. Journal of Chemical Physics, 2005, 122, 014110.	3.0	120
25	Range-separated density-functional theory with random phase approximation applied to noncovalent intermolecular interactions. Journal of Chemical Physics, 2010, 132, 244108.	3.0	119
26	Influence of core-valence separation of electron localization function. Journal of Computational Chemistry, 1997, 18, 1431-1439.	3.3	118
27	Short-range exchange-correlation energy of a uniform electron gas with modified electron-electron interaction. International Journal of Quantum Chemistry, 2004, 100, 1047-1056.	2.0	115
28	Range-separated density-functional theory with the random-phase approximation: Detailed formalism and illustrative applications. Physical Review A, 2010, 82, .	2.5	115
29	Correlation energies for some two- and four-electron systems along the adiabatic connection in density functional theory. Journal of Chemical Physics, 1999, 110, 2828-2835.	3.0	114
30	Contribution to the electron distribution analysis. I. Shell structure of atoms. Journal of Chemical Physics, 1991, 95, 1928-1942.	3.0	112
31	Expression of the exact electron-correlation-energy density functional in terms of first-order density matrices. Physical Review A, 1995, 52, R1805-R1807.	2.5	111
32	Six questions on topology in theoretical chemistry. Computational and Theoretical Chemistry, 2015, 1053, 2-16.	2.5	99
33	Topological Bifurcation Analysis: Electronic Structure of CH5+. Angewandte Chemie International Edition in English, 1997, 36, 2077-2080.	4.4	97
34	On-top pair-density interpretation of spin density functional theory, with applications to magnetism. International Journal of Quantum Chemistry, 1997, 61, 197-205.	2.0	97
35	Adiabatic connection approach to density functional theory of electronic systems. International Journal of Quantum Chemistry, 2003, 93, 166-190.	2.0	87
36	Localization of Electrons in Intermetallic Phases Containing Aluminum. Angewandte Chemie International Edition in English, 1994, 33, 2069-2073.	4.4	85

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37	Closed-shell ring coupled cluster doubles theory with range separation applied on weak intermolecular interactions. Journal of Chemical Physics, 2011, 135, 084119.	3.0	85
38	Validation and assessment of an accurate approach to the correlation problem in density functional theory: The Krigerâ€“Chenâ€“Iafrateâ€“Savin model. Journal of Chemical Physics, 2002, 117, 10465-10473.	3.0	83
39	How electrons guard the space: shape optimization with probability distribution criteria. Theoretical Chemistry Accounts, 2004, 111, 373-380.	1.4	80
40	Prediction Uncertainty of Density Functional Approximations for Properties of Crystals with Cubic Symmetry. Journal of Physical Chemistry A, 2015, 119, 5288-5304.	2.5	78
41	Zur Bindung in Carbosilanen. Angewandte Chemie, 1992, 104, 185-186.	2.0	77
42	A multiconfigurational hybrid density-functional theory. Journal of Chemical Physics, 2012, 137, 044104.	3.0	77
43	Density Functionals for Correlation Energies of Atoms and Molecules. , 1985, , 177-207.		76
44	On the Electronic Structure of (Phosphino)(silyl)carbenes:â€‰ Single-Crystal X-ray Diffraction and ELF Analyses. Journal of the American Chemical Society, 2000, 122, 998-999.	13.7	68
45	On the significance of ELF basins. Journal of Chemical Sciences, 2005, 117, 473-475.	1.5	63
46	Chemische Bindung anschaulich: die Elektronen-Lokalisierungs-Funktion. Chemie in Unserer Zeit, 1997, 31, 110-120.	0.1	62
47	Properties of short-range and long-range correlation energy density functionals from electron-electron coalescence. Physical Review A, 2006, 73, .	2.5	60
48	Die Elektronen-Lokalisierungs-Funktion incloso-Bor-Clustern. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 1993, 619, 437-441.	1.2	56
49	Beyond the Kohnâ€“Sham Determinant. Recent Advances in Computational, 1995, , 129-153.	0.8	53
50	Maximum probability domains from Quantum Monte Carlo calculations. Journal of Computational Chemistry, 2007, 28, 442-454.	3.3	52
51	Fragment-Localized Kohnâ^'Sham Orbitals via a Singles Configuration-Interaction Procedure and Application to Local Properties and Intermolecular Energy Decomposition Analysis. Journal of Chemical Theory and Computation, 2008, 4, 2020-2029.	5.3	51
52	Analytic Models of Domainâ€Averaged Fermi Holes: A New Tool for the Study of the Nature of Chemical Bonds. Chemistry - A European Journal, 2008, 14, 3338-3345.	3.3	43
53	Is size-consistency possible with density functional approximations?. Chemical Physics, 2009, 356, 91-97.	1.9	43
54	The analysis of â€œempty spaceâ€•in the PdGa5 structure. Journal of Alloys and Compounds, 1997, 255, 203-208.	5.5	42

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55	Study of the discontinuity of the exchangeâ€correlation potential in an exactly soluble case. International Journal of Quantum Chemistry, 2009, 109, 2410-2415.	2.0	40
56	Exchangeâ€“Correlation Functionals via Local Interpolation along the Adiabatic Connection. Journal of Chemical Theory and Computation, 2016, 12, 2598-2610.	5.3	40
57	Simple model for the spherically and system-averaged pair density: Results for two-electron atoms. Physical Review A, 2005, 71, .	2.5	38
58	On choosing the best density functional approximation. Chemical Modelling, 0, , 168-185.	0.4	38
59	Exchange-correlation energies and correlation holes for some two- and four-electron atoms along a nonlinear adiabatic connection in density functional theory. International Journal of Quantum Chemistry, 2003, 91, 84-93.	2.0	36
60	Maximal probability domains in linear molecules. Journal of Computational Chemistry, 2005, 26, 455-460.	3.3	36
61	Analysis of the linear response function along the adiabatic connection from the Kohnâ€“Sham to the correlated system. Journal of Chemical Physics, 2001, 115, 6827-6833.	3.0	34
62	Curing basis-set convergence of wave-function theory using density-functional theory: A systematically improvable approach. Journal of Chemical Physics, 2018, 149, 194301.	3.0	33
63	Probabilistic performance estimators for computational chemistry methods: The empirical cumulative distribution function of absolute errors. Journal of Chemical Physics, 2018, 148, 241707.	3.0	32
64	Hohenberg-Kohn theory including spin magnetism and magnetic fields. International Journal of Quantum Chemistry, 2004, 100, 20-21.	2.0	31
65	Constrained-pairing mean-field theory. III. Inclusion of density functional exchange and correlation effects via alternative densities. Journal of Chemical Physics, 2010, 132, 024111.	3.0	30
66	Locally rangeâ€separated hybrids as linear combinations of rangeâ€separated local hybrids. International Journal of Quantum Chemistry, 2009, 109, 2023-2032.	2.0	28
67	An ab initio investigation of the molecules X2, CuX, Cu2X and CuX2 (X = Si, Ge, and Sn). Computational and Theoretical Chemistry, 1995, 339, 67-81.	1.5	24
68	Local density approximation for long-range or for short-range energy functionals?. Computational and Theoretical Chemistry, 2006, 762, 147-150.	1.5	24
69	PROBABILITY DISTRIBUTIONS AND VALENCE SHELLS IN ATOMS. , 2002, , 43-62.		23
70	Electronic excitations from a linear-response range-separated hybrid scheme. Molecular Physics, 2013, 111, 1219-1234.	1.7	23
71	Die Elektronenlokalisierung in aluminiumhaltigen intermetallischen Phasen. Angewandte Chemie, 1994, 106, 2147-2150.	2.0	22
72	Generation and Characterization of Diphosphene and Triphosphene Radical Anions. Computational Studies on the Structure and Stability of P3H3â€¢-Ââ€. Inorganic Chemistry, 1996, 35, 2119-2126.	4.0	22

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73	Maximum Probability Domains in Crystals: The Rock-Salt Structure. Journal of Physical Chemistry A, 2011, 115, 13139-13148.	2.5	22
74	Scaling relations, virial theorem, and energy densities for long-range and short-range density functionals. International Journal of Quantum Chemistry, 2006, 106, 2026-2034.	2.0	21
75	A new Jastrow factor for atoms and molecules, using twoâ€electron systems as a guiding principle. Journal of Chemical Physics, 1995, 103, 691-697.	3.0	20
76	Correlation energy contributions from low-lying states to density functionals based on an electron gas with a gap. International Journal of Quantum Chemistry, 1999, 75, 885-888.	2.0	20
77	Constrained-pairing mean-field theory. IV. Inclusion of corresponding pair constraints and connection to unrestricted Hartreeâ€“Fock theory. Journal of Chemical Physics, 2010, 133, 134108.	3.0	19
78	The Bond Analysis Techniques (ELF and Maximum Probability Domains) Application to a Family of Models Relevant to Bio-Inorganic Chemistry. Structure and Bonding, 2013, , 119-141.	1.0	19
79	Extrapolating the correlation energy. Chemical Physics Letters, 1999, 307, 227-234.	2.6	18
80	Intracule densities in the strong-interaction limit of density functional theory. Physical Chemistry Chemical Physics, 2008, 10, 3440.	2.8	17
81	Excitation energies along a range-separated adiabatic connection. Journal of Chemical Physics, 2014, 141, 044123.	3.0	17
82	Atoms and bonds in molecules and chemical explanations. Foundations of Chemistry, 2014, 16, 3-26.	1.1	17
83	A test for the Wilsonâ€”Levy correlation energy functional. Chemical Physics Letters, 1994, 217, 566-570.	2.6	16
84	Impact of non-normal error distributions on the benchmarking and ranking of quantum machine learning models. Machine Learning: Science and Technology, 2020, 1, 035011.	5.0	16
85	Reduction of the computational effort in quantum Monte Carlo calculations with pseudopotentials through a change of the projection operators. Journal of Chemical Physics, 1992, 97, 459-463.	3.0	14
86	Charge density reconstitution from approximate exchange-correlation holes. Canadian Journal of Chemistry, 2009, 87, 1444-1450.	1.1	14
87	Calculating excitation energies by extrapolation along adiabatic connections. Physical Review A, 2015, 91, .	2.5	14
88	Bounding the extrapolated correlation energy using Padï¿½ approximants. International Journal of Quantum Chemistry, 2000, 79, 222-234.	2.0	13
89	Probabilistic performance estimators for computational chemistry methods: Systematic improvement probability and ranking probability matrix. I. Theory. Journal of Chemical Physics, 2020, 152, 164108.	3.0	13
90	Correlation Contributions from Density Functionals. , 1991, , 213-230.		13

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91	Orbital-Free Embedding Effective Potential in Analytically Solvable Cases. Progress in Theoretical Chemistry and Physics, 2009, , 311-326.	0.2	13
92	A systematic study on the fixed-node and localization error in quantum Monte Carlo calculations with pseudopotentials for group III elements. Chemical Physics Letters, 1994, 222, 274-280.	2.6	12
93	Exchangeâ€“correlation potentials and local energies per particle along nonlinear adiabatic connections. Molecular Physics, 2005, 103, 2725-2734.	1.7	12
94	Maximum Probability Domains in the Solidâ€State Structures of the Elements: the Diamond Structure. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2011, 637, 882-884.	1.2	12
95	Towards a systematic way to correct density functional approximations. Journal of Chemical Physics, 2014, 140, 18A509.	3.0	12
96	Excited states from range-separated density-functional perturbation theory. Molecular Physics, 2015, 113, 1740-1749.	1.7	12
97	Models and corrections: Range separation for electronic interactionâ€”Lessons from density functional theory. Journal of Chemical Physics, 2020, 153, 160901.	3.0	12
98	Range separation combined with the Overhauser model: Application to the H₂ molecule along the dissociation curve. International Journal of Quantum Chemistry, 2009, 109, 1950-1961.	2.0	10
99	Correcting model energies by numerically integrating along an adiabatic connection and a link to density functional approximations. Journal of Chemical Physics, 2011, 134, 214108.	3.0	10
100	Smooth models for the Coulomb potential. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	9
101	Atomic correlation energy differences by means of a polarization potential. Physical Review A, 1988, 38, 483-486.	2.5	8
102	Understanding Maximum Probability Domains with Simple Models. Progress in Theoretical Chemistry and Physics, 2012, , 173-184.	0.2	8
103	Electron affinities of alkaline-earth atoms by means of different density functionals. Physical Review A, 1989, 40, 2163-2165.	2.5	7
104	Topologische Bifurkationsanalyse: Elektronenstruktur von CH₅. Angewandte Chemie, 1997, 109, 2168-2170.	2.0	7
105	Symmetry breaking of relativistic multiconfiguration methods in the nonrelativistic limit. Nonlinearity, 2010, 23, 767-791.	1.4	7
106	On the Use of Benchmarks for Multiple Properties. Computation, 2016, 4, 20.	2.0	7
107	Alternative Representations of the Correlation Energy in Densityâ€Functional Theory: A Kineticâ€Energy Based Adiabatic Connection. Journal of the Chinese Chemical Society, 2016, 63, 121-128.	1.4	7
108	Probabilistic performance estimators for computational chemistry methods: Systematic improvement probability and ranking probability matrix. II. Applications. Journal of Chemical Physics, 2020, 152, 164109.	3.0	7

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109	Transfer of electron correlation from an electron gas to inhomogeneous systems via Jastrow factors. Physical Review A, 1994, 50, 3742-3746.	2.5	6
110	High-Density Limit of Two-Electron Systems:â€‰ Results from the Extended Overhauser Approach. Journal of Chemical Theory and Computation, 2007, 3, 796-802.	5.3	5
111	When does a functional correctly describe both the structure and the energy of the transition state?. Journal of Molecular Modeling, 2017, 23, 65.	1.8	5
112	Excitation energies from GÃ¶rlingâ€“Levy perturbation theory along the range-separated adiabatic connection. Molecular Physics, 2018, 116, 1443-1451.	1.7	5
113	Using the Gini coefficient to characterize the shape of computational chemistry error distributions. Theoretical Chemistry Accounts, 2021, 140, 1.	1.4	5
114	Acknowledging User Requirements for Accuracy in Computational Chemistry Benchmarks. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2020, 646, 1042-1045.	1.2	4
115	Adiabatic Coupling in the Helium and the Beryllium Series. , 1998, , 69-80.		4
116	Chemical Bonding and Interpretation of Time-Dependent Electronic Processes with Maximum Probability Domains. Wuli Huaxue Xuebao/ Acta Physico - Chimica Sinica, 2018, 34, 528-536.	4.9	4
117	Full configuration interaction wave function as a formal solution to the optimized effective potential and Kohnâ€“Sham models in finite basis sets. Computational and Theoretical Chemistry, 2010, 943, 90-93.	1.5	3
118	Maximum probability domains for the analysis of the microscopic structure of liquids. Journal of Chemical Physics, 2015, 142, 064117.	3.0	3
119	Absence of proof for the Hohenbergâ€“Kohn theorem for a Hamiltonian linear in the magnetic field. Molecular Physics, 2017, 115, 13-15.	1.7	3
120	Was Pauling Mistaken about Metals?. Molecules, 2021, 26, 1930.	3.8	3
121	A spectral analysis of the correlation energy. Computational and Theoretical Chemistry, 2000, 527, 121-125.	1.5	2
122	Potential-Driven Adiabatic Connection in Density Functional Theory. Journal of Chemical Theory and Computation, 2009, 5, 822-826.	5.3	2
123	Range-separated density-functional theory applied to the beryllium dimer and trimer. Theoretical Chemistry Accounts, 2018, 137, 1.	1.4	2
124	Challenges for large scale simulation: general discussion. Faraday Discussions, 2020, 224, 309-332.	3.2	2
125	Strong correlation in density functional theory: general discussion. Faraday Discussions, 2020, 224, 373-381.	3.2	2
126	New approaches to study excited states in density functional theory: general discussion. Faraday Discussions, 2020, 224, 483-508.	3.2	2

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127	Should We Gain Confidence from the Similarity of Results between Methods?. Computation, 2022, 10, 27.	2.0	2
128	Two-particle coalescence conditions revisited. Molecular Physics, 2022, 120, .	1.7	2
129	The effect of uncertainty on building blocks in molecules. Journal of Chemical Physics, 2022, 156, .	3.0	2
130	New density-functional approximations and beyond: general discussion. Faraday Discussions, 2020, 224, 166-200.	3.2	1
131	Concluding remarks for the new horizons in density functional theory Faraday Discussion. Faraday Discussions, 2020, 224, 509-514.	3.2	1