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	Should We Gain Confidence from the Similarity of Results between Methods?. Computation, 2022, 10, 27.	2.0	2
2	Two-particle coalescence conditions revisited. Molecular Physics, 2022, 120, .	1.7	2
3	The effect of uncertainty on building blocks in molecules. Journal of Chemical Physics, 2022, 156, .	3.0	2
4	Using the Gini coefficient to characterize the shape of computational chemistry error distributions. Theoretical Chemistry Accounts, 2021, 140, 1.	1.4	5
5	Was Pauling Mistaken about Metals?. Molecules, 2021, 26, 1930.	3.8	3
6	Challenges for large scale simulation: general discussion. Faraday Discussions, 2020, 224, 309-332.	3.2	2
7	New density-functional approximations and beyond: general discussion. Faraday Discussions, 2020, 224, 166-200.	3.2	1
8	Strong correlation in density functional theory: general discussion. Faraday Discussions, 2020, 224, 373-381.	3.2	2
9	New approaches to study excited states in density functional theory: general discussion. Faraday Discussions, 2020, 224, 483-508.	3.2	2
10	Concluding remarks for the new horizons in density functional theory Faraday Discussion. Faraday Discussions, 2020, 224, 509-514.	3.2	1
11	Models and corrections: Range separation for electronic interactionâ€"Lessons from density functional theory. Journal of Chemical Physics, 2020, 153, 160901.	3.0	12
12	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
13	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
14	Acknowledging User Requirements for Accuracy in Computational Chemistry Benchmarks. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2020, 646, 1042-1045.	1.2	4
15	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
16	Excitation energies from GÃ¶rlingâ€"Levy perturbation theory along the range-separated adiabatic connection. Molecular Physics, 2018, 116, 1443-1451.	1.7	5
17	Range-separated density-functional theory applied to the beryllium dimer and trimer. Theoretical Chemistry Accounts, 2018, 137, 1.	1.4	2
18	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

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19	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
20	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
21	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
22	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
23	On the Use of Benchmarks for Multiple Properties. Computation, 2016, 4, 20.	2.0	7
24	Exchangeâ€“Correlation Functionals via Local Interpolation along the Adiabatic Connection. Journal of Chemical Theory and Computation, 2016, 12, 2598-2610.	5.3	40
25	Smooth models for the Coulomb potential. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	9
26	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
27	Excited states from range-separated density-functional perturbation theory. Molecular Physics, 2015, 113, 1740-1749.	1.7	12
28	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
29	Calculating excitation energies by extrapolation along adiabatic connections. Physical Review A, 2015, 91, .	2.5	14
30	Maximum probability domains for the analysis of the microscopic structure of liquids. Journal of Chemical Physics, 2015, 142, 064117.	3.0	3
31	Six questions on topology in theoretical chemistry. Computational and Theoretical Chemistry, 2015, 1053, 2-16.	2.5	99
32	Towards a systematic way to correct density functional approximations. Journal of Chemical Physics, 2014, 140, 18A509.	3.0	12
33	Excitation energies along a range-separated adiabatic connection. Journal of Chemical Physics, 2014, 141, 044123.	3.0	17
34	Atoms and bonds in molecules and chemical explanations. Foundations of Chemistry, 2014, 16, 3-26.	1.1	17
35	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
36	Electronic excitations from a linear-response range-separated hybrid scheme. Molecular Physics, 2013, 111, 1219-1234.	1.7	23

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37	A multiconfigurational hybrid density-functional theory. Journal of Chemical Physics, 2012, 137, 044104.	3.0	77
38	Understanding Maximum Probability Domains with Simple Models. Progress in Theoretical Chemistry and Physics, 2012, , 173-184.	0.2	8
39	Maximum Probability Domains in Crystals: The Rock-Salt Structure. Journal of Physical Chemistry A, 2011, 115, 13139-13148.	2.5	22
40	Double-hybrid density-functional theory made rigorous. Journal of Chemical Physics, 2011, 134, 064113.	3.0	165
41	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
42	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
43	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
44	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
45	Symmetry breaking of relativistic multiconfiguration methods in the nonrelativistic limit. Nonlinearity, 2010, 23, 767-791.	1.4	7
46	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
47	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
48	Range-separated density-functional theory with random phase approximation applied to noncovalent intermolecular interactions. Journal of Chemical Physics, 2010, 132, 244108.	3.0	119
49	Range-separated density-functional theory with the random-phase approximation: Detailed formalism and illustrative applications. Physical Review A, 2010, 82, .	2.5	115
50	Adiabatic-Connection Fluctuation-Dissipation Density-Functional Theory Based on Range Separation. Physical Review Letters, 2009, 102, 096404.	7.8	240
51	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
52	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
53	Locally rangeâ€separated hybrids as linear combinations of rangeâ€separated local hybrids. International Journal of Quantum Chemistry, 2009, 109, 2023-2032.	2.0	28
54	Is size-consistency possible with density functional approximations?. Chemical Physics, 2009, 356, 91-97.	1.9	43

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55	Potential-Driven Adiabatic Connection in Density Functional Theory. Journal of Chemical Theory and Computation, 2009, 5, 822-826.	5.3	2
56	Charge density reconstitution from approximate exchange-correlation holes. Canadian Journal of Chemistry, 2009, 87, 1444-1450.	1.1	14
57	Orbital-Free Embedding Effective Potential in Analytically Solvable Cases. Progress in Theoretical Chemistry and Physics, 2009, , 311-326.	0.2	13
58	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
59	Intracule densities in the strong-interaction limit of density functional theory. Physical Chemistry Chemical Physics, 2008, 10, 3440.	2.8	17
60	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
61	Assessment of a Middle-Range Hybrid Functional. Journal of Chemical Theory and Computation, 2008, 4, 1254-1262.	5.3	155
62	Hybrid functionals with local range separation. Journal of Chemical Physics, 2008, 129, 124103.	3.0	134
63	The importance of middle-range Hartree-Fock-type exchange for hybrid density functionals. Journal of Chemical Physics, 2007, 127, 221103.	3.0	152
64	Strictly correlated electrons in density-functional theory: A general formulation with applications to spherical densities. Physical Review A, 2007, 75, .	2.5	126
65	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
66	Maximum probability domains from Quantum Monte Carlo calculations. Journal of Computational Chemistry, 2007, 28, 442-454.	3.3	52
67	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
68	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
69	Local density approximation for long-range or for short-range energy functionals?. Computational and Theoretical Chemistry, 2006, 762, 147-150.	1.5	24
70	Properties of short-range and long-range correlation energy density functionals from electron-electron coalescence. Physical Review A, 2006, 73, .	2.5	60
71	The electron localization function (ELF) and its relatives: interpretations and difficulties. Computational and Theoretical Chemistry, 2005, 727, 127-131.	1.5	144
72	Maximal probability domains in linear molecules. Journal of Computational Chemistry, 2005, 26, 455-460.	3.3	36

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73	On the significance of ELF basins. Journal of Chemical Sciences, 2005, 117, 473-475.	1.5	63
74	Simple model for the spherically and system-averaged pair density: Results for two-electron atoms. Physical Review A, 2005, 71, .	2.5	38
75	Exchangeâ€“correlation potentials and local energies per particle along nonlinear adiabatic connections. Molecular Physics, 2005, 103, 2725-2734.	1.7	12
76	Short-range exchange and correlation energy density functionals: Beyond the local-density approximation. Journal of Chemical Physics, 2005, 122, 014110.	3.0	120
77	van der Waals forces in density functional theory: Perturbational long-range electron-interaction corrections. Physical Review A, 2005, 72, .	2.5	287
78	How electrons guard the space: shape optimization with probability distribution criteria. Theoretical Chemistry Accounts, 2004, 111, 373-380.	1.4	80
79	Hohenberg-Kohn theory including spin magnetism and magnetic fields. International Journal of Quantum Chemistry, 2004, 100, 20-21.	2.0	31
80	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
81	Long-rangeâ€“short-range separation of the electron-electron interaction in density-functional theory. Physical Review A, 2004, 70, .	2.5	381
82	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
83	Adiabatic connection approach to density functional theory of electronic systems. International Journal of Quantum Chemistry, 2003, 93, 166-190.	2.0	87
84	PROBABILITY DISTRIBUTIONS AND VALENCE SHELLS IN ATOMS. , 2002, , 43-62.		23
85	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
86	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
87	Bounding the extrapolated correlation energy using Padï¿½ approximants. International Journal of Quantum Chemistry, 2000, 79, 222-234.	2.0	13
88	A spectral analysis of the correlation energy. Computational and Theoretical Chemistry, 2000, 527, 121-125.	1.5	2
89	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
90	Extrapolating the correlation energy. Chemical Physics Letters, 1999, 307, 227-234.	2.6	18

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91	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
92	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
93	Construction of An Accurate Self-interaction-corrected Correlation Energy Functional Based on An Electron Gas with A Gap. , 1999, , 463-477.		122
94	Virtual space level shifting and correlation energies. International Journal of Quantum Chemistry, 1998, 69, 581-590.	2.0	143
95	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
96	Adiabatic Coupling in the Helium and the Beryllium Series. , 1998, , 69-80.		4
97	A correlation-energy density functional for multideterminantal wavefunctions. Molecular Physics, 1997, 91, 527-536.	1.7	149
98	The analysis of â€œempty spaceâ€•in the PdGa5 structure. Journal of Alloys and Compounds, 1997, 255, 203-208.	5.5	42
99	ELF: The Electron Localization Function. Angewandte Chemie International Edition in English, 1997, 36, 1808-1832.	4.4	1,929
100	Topological Bifurcation Analysis: Electronic Structure of CH5+. Angewandte Chemie International Edition in English, 1997, 36, 2077-2080.	4.4	97
101	Die Elektronenlokalisierungsfunktion ELF. Angewandte Chemie, 1997, 109, 1892-1918.	2.0	190
102	Topologische Bifurkationsanalyse: Elektronenstruktur von CH₅. Angewandte Chemie, 1997, 109, 2168-2170.	2.0	7
103	Chemische Bindung anschaulich: die Elektronen-Lokalisierungs-Funktion. Chemie in Unserer Zeit, 1997, 31, 110-120.	0.1	62
104	Influence of core-valence separation of electron localization function. Journal of Computational Chemistry, 1997, 18, 1431-1439.	3.3	118
105	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
106	Combining long-range configuration interaction with short-range density functionals. Chemical Physics Letters, 1997, 275, 151-160.	2.6	681
107	Generation and Characterization of Diphosphene and Triphosphene Radical Anions. Computational Studies on the Structure and Stability of P3H3â€¢-Âã€. Inorganic Chemistry, 1996, 35, 2119-2126.	4.0	22
108	Beyond the Kohnâ€“Sham Determinant. Recent Advances in Computational, 1995, , 129-153.	0.8	53

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109	Density functionals for the Yukawa electron-electron interaction. International Journal of Quantum Chemistry, 1995, 56, 327-332.	2.0	261
110	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
111	Escaping the symmetry dilemma through a pair-density interpretation of spin-density functional theory. Physical Review A, 1995, 51, 4531-4541.	2.5	335
112	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
113	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
114	Transfer of electron correlation from an electron gas to inhomogeneous systems via Jastrow factors. Physical Review A, 1994, 50, 3742-3746.	2.5	6
115	A test for the Wilsonâ€”Levy correlation energy functional. Chemical Physics Letters, 1994, 217, 566-570.	2.6	16
116	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
117	Localization of Electrons in Intermetallic Phases Containing Aluminum. Angewandte Chemie International Edition in English, 1994, 33, 2069-2073.	4.4	85
118	Die Elektronenlokalisierung in aluminiumhaltigen intermetallischen Phasen. Angewandte Chemie, 1994, 106, 2147-2150.	2.0	22
119	Die Elektronen-Lokalisierungs-Funktion incloso-Bor-Clustern. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 1993, 619, 437-441.	1.2	56
120	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
121	On the Bonding in Carbosilanes. Angewandte Chemie International Edition in English, 1992, 31, 185-187.	4.4	137
122	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
123	Zur Bindung in Carbosilanen. Angewandte Chemie, 1992, 104, 185-186.	2.0	77
124	Die Elektronenlokalisierung in den FestkÃ¶rperâ€strukturen der Elemente: die Diamantstruktur. Angewandte Chemie, 1992, 104, 186-188.	2.0	121
125	Contribution to the electron distribution analysis. I. Shell structure of atoms. Journal of Chemical Physics, 1991, 95, 1928-1942.	3.0	112
126	Correlation Contributions from Density Functionals. , 1991, , 213-230.		13

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127	Electron affinities of alkaline-earth atoms by means of different density functionals. Physical Review A, 1989, 40, 2163-2165.	2.5	7
128	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
129	Atomic correlation energy differences by means of a polarization potential. Physical Review A, 1988, 38, 483-486.	2.5	8
130	Density Functionals for Correlation Energies of Atoms and Molecules. , 1985, , 177-207.		76
131	On choosing the best density functional approximation. Chemical Modelling, 0, , 168-185.	0.4	38