Axel D Becke

List of Publications by Year
in descending order

54 papers	116,916 citations	159585 30 h-index	161849 54 g-index
54 all docs	54 docs citations	54 times ranked	66032 citing authors

#	Article	IF	Citations
1	Densityâ€functional thermochemistry. III. The role of exact exchange. Journal of Chemical Physics, 1993, 98, 5648-5652.	3.0	91,707
2	A new mixing of Hartreeâ€“Fock and local densityâ€functional theories. Journal of Chemical Physics, 1993, 98, 1372-1377.	3.0	14,273
3	Density-functional thermochemistry. V. Systematic optimization of exchange-correlation functionals. Journal of Chemical Physics, 1997, 107, 8554-8560.	3.0	1,673
4	A simple effective potential for exchange. Journal of Chemical Physics, 2006, 124, 221101.	3.0	1,200
5	A density-functional model of the dispersion interaction. Journal of Chemical Physics, 2005, 123, 154101.	3.0	1,150
6	Perspective: Fifty years of density-functional theory in chemical physics. Journal of Chemical Physics, 2014, 140, 18A301.	3.0	1,083
7	A post-Hartree-Fock model of intermolecular interactions: Inclusion of higher-order corrections. Journal of Chemical Physics, 2006, 124, 174104.	3.0	896
8	A post-Hartreeâ€“Fock model of intermolecular interactions. Journal of Chemical Physics, 2005, 123, 024101.	3.0	735
9	Optimized density functionals from the extended G2 test set. Journal of Chemical Physics, 1998, 108, 9624-9631.	3.0	694
10	Exchange-hole dipole moment and the dispersion interaction. Journal of Chemical Physics, 2005, 122, 154104.	3.0	497
11	Exchange-hole dipole moment and the dispersion interaction revisited. Journal of Chemical Physics, 2007, 127, 154108.	3.0	432
12	Real-space post-Hartreeâ€“Fock correlation models. Journal of Chemical Physics, 2005, 122, 064101.	3.0	231
13	A real-space model of nondynamical correlation. Journal of Chemical Physics, 2003, 119, 2972-2977.	3.0	200
14	A unified density-functional treatment of dynamical, nondynamical, and dispersion correlations. Journal of Chemical Physics, 2007, 127, 124108.	3.0	193
15	Exchange-hole dipole moment and the dispersion interaction: High-order dispersion coefficients. Journal of Chemical Physics, 2006, 124, 014104.	3.0	184
16	Simulation of delocalized exchange by local density functionals. Journal of Chemical Physics, 2000, 112, 4020-4026.	3.0	165
17	van der Waals Interactions in Density-Functional Theory: Intermolecular Complexes. Journal of Chemical Theory and Computation, 2010, 6, 1081-1088.	5.3	155
18	Oscillations in meta-generalized-gradient approximation potential energy surfaces for dispersion-bound complexes. Journal of Chemical Physics, 2009, 131, 034111.	3.0	153

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19	Van der Waals Interactions in Density-Functional Theory: Rare-Gas Diatomics. Journal of Chemical Theory and Computation, 2009, 5, 719-727.	5.3	145
20	Density functionals for static, dynamical, and strong correlation. Journal of Chemical Physics, 2013, 138, 074109.	3.0	144
21	Current density in exchange-correlation functionals: Application to atomic states. Journal of Chemical Physics, 2002, 117, 6935-6938.	3.0	102
22	Exploring the limits of gradient corrections in density functional theory. Journal of Computational Chemistry, 1999, 20, 63-69.	3.3	83
23	Thermochemical tests of a kinetic-energy dependent exchange-correlation approximation. International Journal of Quantum Chemistry, 1994, 52, 625-632.	2.0	81
24	EXCHANGEâ€“CORRELATION APPROXIMATIONS IN DENSITY-FUNCTIONAL THEORY. Advanced Series in Physical Chemistry, 1995, , 1022-1046.	1.5	61
25	Van der Waals interactions from the exchange hole dipole moment: Application to bio-organic benchmark systems. Chemical Physics Letters, 2006, 432, 600-603.	2.6	61
26	Current-density dependent exchange-correlation functionals. Canadian Journal of Chemistry, 1996, 74, 995-997.	1.1	60
27	Pervasive Delocalisation Error Causes Spurious Proton Transfer in Organic Acidâ€“Base Coâ€€Crystals. Angewandte Chemie - International Edition, 2018, 57, 14906-14910.	13.8	45
28	Communication: DFT treatment of strong correlation in 3d transition-metal diatomics. Journal of Chemical Physics, 2017, 146, 211105.	3.0	42
29	Local Density-Functional Polarizabilities and Hyperpolarizabilities at the Basis-Set Limit. The Journal of Physical Chemistry, 1996, 100, 16105-16108.	2.9	40
30	A unified density-functional treatment of dynamical, nondynamical, and dispersion correlations. II. Thermochemical and kinetic benchmarks. Journal of Chemical Physics, 2008, 128, 124105.	3.0	39
31	Quantum Chemical Methods for Modeling Covalent Modification of Biological Thiols. Journal of Computational Chemistry, 2020, 41, 427-438.	3.3	31
32	Density functionals and transition-metal atoms. Journal of Chemical Physics, 2007, 126, 184104.	3.0	29
33	Atomic volumes and polarizabilities in density-functional theory. Journal of Chemical Physics, 2012, 136, 034109.	3.0	29
34	Nonempirical density-functional theory for van der Waals interactions. Canadian Journal of Chemistry, 2010, 88, 1057-1062.	1.1	27
35	Communication: Calibration of a strong-correlation density functional on transition-metal atoms. Journal of Chemical Physics, 2013, 138, 161101.	3.0	26
36	Tests of an exact-exchange-based density-functional theory on transition-metal complexes. Canadian Journal of Chemistry, 2009, 87, 1369-1373.	1.1	24

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37	Vertical excitation energies from the adiabatic connection. Journal of Chemical Physics, 2016, 145, 194107.	3.0	24
38	Basis-set-free density-functional quantum chemistry. International Journal of Quantum Chemistry, 1989, 36, 599-609.	2.0	23
39	Communication: Two-determinant mixing with a strong-correlation density functional. Journal of Chemical Physics, 2013, 139, 021104.	3.0	21
40	Communication: Correct charge transfer in CT complexes from the Beckeâ€™05 density functional. Journal of Chemical Physics, 2018, 148, 211101.	3.0	20
41	Singlet-triplet splittings from the virial theorem and single-particle excitation energies. Journal of Chemical Physics, 2018, 148, 044112.	3.0	19
42	Density-functional theory vs density-functional fits. Journal of Chemical Physics, 2022, 156, .	3.0	19
43	Interrogating the Beckeâ€™05 density functional for non-locality information. Journal of Chemical Physics, 2017, 147, 154103.	3.0	15
44	Assessment of the PW86+PBE+XDM density functional on van der Waals complexes at non-equilibrium geometries. Journal of Chemical Physics, 2012, 137, 014104.	3.0	14
45	Communication: Optical gap in polyacetylene from a simple quantum chemistry exciton model. Journal of Chemical Physics, 2018, 149, 081102.	3.0	11
46	Pervasive Delocalisation Error Causes Spurious Proton Transfer in Organic Acidâ€“Base Coâ€Crystals. Angewandte Chemie, 2018, 130, 15122-15126.	2.0	10
47	Density-functional description of alkalides: introducing the alkalide state. Physical Chemistry Chemical Physics, 2018, 20, 26710-26718.	2.8	9
48	Communication: Beckeâ€™s virial exciton model gives accurate charge-transfer excitation energies. Journal of Chemical Physics, 2018, 149, 231101.	3.0	9
49	Theoretical investigation of polymorph- and coformer-dependent photoluminescence in molecular crystals. CrystEngComm, 2021, 23, 4264-4271.	2.6	9
50	A density-functional approximation for relativistic kinetic energy. Journal of Chemical Physics, 2009, 131, 244118.	3.0	6
51	Fractional Kohnâ€“Sham Occupancies from a Strong-Correlation Density Functional. Topics in Current Chemistry, 2014, , 175-186.	4.0	6
52	Excited-state surfaces of ethylene from the B13 strong-correlation density functional. Molecular Physics, 2015, 113, 1884-1889.	1.7	6
53	Computational modeling of piezochromism in molecular crystals. Journal of Chemical Physics, 2020, 152, 234106.	3.0	4
54	Dependence of the virial exciton model on basis set and exact-exchange fraction. Journal of Chemical Physics, 2019, 150, 241101.	3.0	1