

Axel D Becke

List of Publications by Year in descending order

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54
papers

116,916
citations

159358

30
h-index

161609

54
g-index

54
all docs

54
docs citations

54
times ranked

66032
citing authors

#	ARTICLE	IF	CITATIONS
1	Density-functional thermochemistry. III. The role of exact exchange. <i>Journal of Chemical Physics</i> , 1993, 98, 5648-5652.	1.2	91,707
2	A new mixing of Hartree-Fock and local density-functional theories. <i>Journal of Chemical Physics</i> , 1993, 98, 1372-1377.	1.2	14,273
3	Density-functional thermochemistry. V. Systematic optimization of exchange-correlation functionals. <i>Journal of Chemical Physics</i> , 1997, 107, 8554-8560.	1.2	1,673
4	A simple effective potential for exchange. <i>Journal of Chemical Physics</i> , 2006, 124, 221101.	1.2	1,200
5	A density-functional model of the dispersion interaction. <i>Journal of Chemical Physics</i> , 2005, 123, 154101.	1.2	1,150
6	Perspective: Fifty years of density-functional theory in chemical physics. <i>Journal of Chemical Physics</i> , 2014, 140, 18A301.	1.2	1,083
7	A post-Hartree-Fock model of intermolecular interactions: Inclusion of higher-order corrections. <i>Journal of Chemical Physics</i> , 2006, 124, 174104.	1.2	896
8	A post-Hartree-Fock model of intermolecular interactions. <i>Journal of Chemical Physics</i> , 2005, 123, 024101.	1.2	735
9	Optimized density functionals from the extended G2 test set. <i>Journal of Chemical Physics</i> , 1998, 108, 9624-9631.	1.2	694
10	Exchange-hole dipole moment and the dispersion interaction. <i>Journal of Chemical Physics</i> , 2005, 122, 154104.	1.2	497
11	Exchange-hole dipole moment and the dispersion interaction revisited. <i>Journal of Chemical Physics</i> , 2007, 127, 154108.	1.2	432
12	Real-space post-Hartree-Fock correlation models. <i>Journal of Chemical Physics</i> , 2005, 122, 064101.	1.2	231
13	A real-space model of nondynamical correlation. <i>Journal of Chemical Physics</i> , 2003, 119, 2972-2977.	1.2	200
14	A unified density-functional treatment of dynamical, nondynamical, and dispersion correlations. <i>Journal of Chemical Physics</i> , 2007, 127, 124108.	1.2	193
15	Exchange-hole dipole moment and the dispersion interaction: High-order dispersion coefficients. <i>Journal of Chemical Physics</i> , 2006, 124, 014104.	1.2	184
16	Simulation of delocalized exchange by local density functionals. <i>Journal of Chemical Physics</i> , 2000, 112, 4020-4026.	1.2	165
17	van der Waals Interactions in Density-Functional Theory: Intermolecular Complexes. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 1081-1088.	2.3	155
18	Oscillations in meta-generalized-gradient approximation potential energy surfaces for dispersion-bound complexes. <i>Journal of Chemical Physics</i> , 2009, 131, 034111.	1.2	153

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19	Van der Waals Interactions in Density-Functional Theory: Rare-Gas Diatomics. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 719-727.	2.3	145
20	Density functionals for static, dynamical, and strong correlation. <i>Journal of Chemical Physics</i> , 2013, 138, 074109.	1.2	144
21	Current density in exchange-correlation functionals: Application to atomic states. <i>Journal of Chemical Physics</i> , 2002, 117, 6935-6938.	1.2	102
22	Exploring the limits of gradient corrections in density functional theory. <i>Journal of Computational Chemistry</i> , 1999, 20, 63-69.	1.5	83
23	Thermochemical tests of a kinetic-energy dependent exchange-correlation approximation. <i>International Journal of Quantum Chemistry</i> , 1994, 52, 625-632.	1.0	81
24	EXCHANGE-CORRELATION APPROXIMATIONS IN DENSITY-FUNCTIONAL THEORY. <i>Advanced Series in Physical Chemistry</i> , 1995, , 1022-1046.	1.5	61
25	Van der Waals interactions from the exchange hole dipole moment: Application to bio-organic benchmark systems. <i>Chemical Physics Letters</i> , 2006, 432, 600-603.	1.2	61
26	Current-density dependent exchange-correlation functionals. <i>Canadian Journal of Chemistry</i> , 1996, 74, 995-997.	0.6	60
27	Pervasive Delocalisation Error Causes Spurious Proton Transfer in Organic Acid-Base Crystals. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 14906-14910.	7.2	45
28	Communication: DFT treatment of strong correlation in 3d transition-metal diatomics. <i>Journal of Chemical Physics</i> , 2017, 146, 211105.	1.2	42
29	Local Density-Functional Polarizabilities and Hyperpolarizabilities at the Basis-Set Limit. <i>The Journal of Physical Chemistry</i> , 1996, 100, 16105-16108.	2.9	40
30	A unified density-functional treatment of dynamical, nondynamical, and dispersion correlations. II. Thermochemical and kinetic benchmarks. <i>Journal of Chemical Physics</i> , 2008, 128, 124105.	1.2	39
31	Quantum Chemical Methods for Modeling Covalent Modification of Biological Thiols. <i>Journal of Computational Chemistry</i> , 2020, 41, 427-438.	1.5	31
32	Density functionals and transition-metal atoms. <i>Journal of Chemical Physics</i> , 2007, 126, 184104.	1.2	29
33	Atomic volumes and polarizabilities in density-functional theory. <i>Journal of Chemical Physics</i> , 2012, 136, 034109.	1.2	29
34	Nonempirical density-functional theory for van der Waals interactions. <i>Canadian Journal of Chemistry</i> , 2010, 88, 1057-1062.	0.6	27
35	Communication: Calibration of a strong-correlation density functional on transition-metal atoms. <i>Journal of Chemical Physics</i> , 2013, 138, 161101.	1.2	26
36	Tests of an exact-exchange-based density-functional theory on transition-metal complexes. <i>Canadian Journal of Chemistry</i> , 2009, 87, 1369-1373.	0.6	24

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37	Vertical excitation energies from the adiabatic connection. <i>Journal of Chemical Physics</i> , 2016, 145, 194107.	1.2	24
38	Basis-set-free density-functional quantum chemistry. <i>International Journal of Quantum Chemistry</i> , 1989, 36, 599-609.	1.0	23
39	Communication: Two-determinant mixing with a strong-correlation density functional. <i>Journal of Chemical Physics</i> , 2013, 139, 021104.	1.2	21
40	Communication: Correct charge transfer in CT complexes from the Becke's ω B97X density functional. <i>Journal of Chemical Physics</i> , 2018, 148, 211101.	1.2	20
41	Singlet-triplet splittings from the virial theorem and single-particle excitation energies. <i>Journal of Chemical Physics</i> , 2018, 148, 044112.	1.2	19
42	Density-functional theory vs density-functional fits. <i>Journal of Chemical Physics</i> , 2022, 156, .	1.2	19
43	Interrogating the Becke's ω B97X density functional for non-locality information. <i>Journal of Chemical Physics</i> , 2017, 147, 154103.	1.2	15
44	Assessment of the PW86+PBE+XDM density functional on van der Waals complexes at non-equilibrium geometries. <i>Journal of Chemical Physics</i> , 2012, 137, 014104.	1.2	14
45	Communication: Optical gap in polyacetylene from a simple quantum chemistry exciton model. <i>Journal of Chemical Physics</i> , 2018, 149, 081102.	1.2	11
46	Pervasive Delocalisation Error Causes Spurious Proton Transfer in Organic Acid-Base Crystals. <i>Angewandte Chemie</i> , 2018, 130, 15122-15126.	1.6	10
47	Density-functional description of alkalides: introducing the alkalide state. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 26710-26718.	1.3	9
48	Communication: Becke's ω B97X's virial exciton model gives accurate charge-transfer excitation energies. <i>Journal of Chemical Physics</i> , 2018, 149, 231101.	1.2	9
49	Theoretical investigation of polymorph- and cofomer-dependent photoluminescence in molecular crystals. <i>CrystEngComm</i> , 2021, 23, 4264-4271.	1.3	9
50	A density-functional approximation for relativistic kinetic energy. <i>Journal of Chemical Physics</i> , 2009, 131, 244118.	1.2	6
51	Fractional Kohn-Sham Occupancies from a Strong-Correlation Density Functional. <i>Topics in Current Chemistry</i> , 2014, , 175-186.	4.0	6
52	Excited-state surfaces of ethylene from the B13 strong-correlation density functional. <i>Molecular Physics</i> , 2015, 113, 1884-1889.	0.8	6
53	Computational modeling of piezochromism in molecular crystals. <i>Journal of Chemical Physics</i> , 2020, 152, 234106.	1.2	4
54	Dependence of the virial exciton model on basis set and exact-exchange fraction. <i>Journal of Chemical Physics</i> , 2019, 150, 241101.	1.2	1