Axel D Becke

List of Publications by Year
in descending order

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54 papers	116,916 citations	182225 30 h-index	182931 54 g-index
54 all docs	54 docs citations	54 times ranked	73624 citing authors

#	Article	IF	Citations
1	Density-functional theory vs density-functional fits. Journal of Chemical Physics, 2022, 156, .	1.2	19
2	Theoretical investigation of polymorph- and coformer-dependent photoluminescence in molecular crystals. CrystEngComm, 2021, 23, 4264-4271.	1.3	9
3	Quantum Chemical Methods for Modeling Covalent Modification of Biological Thiols. Journal of Computational Chemistry, 2020, 41, 427-438.	1.5	31
4	Computational modeling of piezochromism in molecular crystals. Journal of Chemical Physics, 2020, 152, 234106.	1.2	4
5	Dependence of the virial exciton model on basis set and exact-exchange fraction. Journal of Chemical Physics, 2019, 150, 241101.	1.2	1
6	Singlet-triplet splittings from the virial theorem and single-particle excitation energies. Journal of Chemical Physics, 2018, 148, 044112.	1.2	19
7	Density-functional description of alkalides: introducing the alkalide state. Physical Chemistry Chemical Physics, 2018, 20, 26710-26718.	1.3	9
8	Communication: Beckeâ€™s virial exciton model gives accurate charge-transfer excitation energies. Journal of Chemical Physics, 2018, 149, 231101.	1.2	9
9	Pervasive Delocalisation Error Causes Spurious Proton Transfer in Organic Acidâ€“Base Coâ€Crystals. Angewandte Chemie, 2018, 130, 15122-15126.	1.6	10
10	Pervasive Delocalisation Error Causes Spurious Proton Transfer in Organic Acidâ€“Base Coâ€Crystals. Angewandte Chemie - International Edition, 2018, 57, 14906-14910.	7.2	45
11	Communication: Optical gap in polyacetylene from a simple quantum chemistry exciton model. Journal of Chemical Physics, 2018, 149, 081102.	1.2	11
12	Communication: Correct charge transfer in CT complexes from the Beckeâ€™05 density functional. Journal of Chemical Physics, 2018, 148, 211101.	1.2	20
13	Interrogating the Beckeâ€™05 density functional for non-locality information. Journal of Chemical Physics, 2017, 147, 154103.	1.2	15
14	Communication: DFT treatment of strong correlation in 3d transition-metal diatomics. Journal of Chemical Physics, 2017, 146, 211105.	1.2	42
15	Vertical excitation energies from the adiabatic connection. Journal of Chemical Physics, 2016, 145, 194107.	1.2	24
16	Excited-state surfaces of ethylene from the B13 strong-correlation density functional. Molecular Physics, 2015, 113, 1884-1889.	0.8	6
17	Fractional Kohnâ€“Sham Occupancies from a Strong-Correlation Density Functional. Topics in Current Chemistry, 2014, , 175-186.	4.0	6
18	Perspective: Fifty years of density-functional theory in chemical physics. Journal of Chemical Physics, 2014, 140, 18A301.	1.2	1,083

#	Article	IF	Citations
19	Communication: Calibration of a strong-correlation density functional on transition-metal atoms. Journal of Chemical Physics, 2013, 138, 161101.	1.2	26
20	Density functionals for static, dynamical, and strong correlation. Journal of Chemical Physics, 2013, 138, 074109.	1.2	144
21	Communication: Two-determinant mixing with a strong-correlation density functional. Journal of Chemical Physics, 2013, 139, 021104.	1.2	21
22	Atomic volumes and polarizabilities in density-functional theory. Journal of Chemical Physics, 2012, 136, 034109.	1.2	29
23	Assessment of the PW86+PBE+XDM density functional on van der Waals complexes at non-equilibrium geometries. Journal of Chemical Physics, 2012, 137, 014104.	1.2	14
24	Nonempirical density-functional theory for van der Waals interactions. Canadian Journal of Chemistry, 2010, 88, 1057-1062.	0.6	27
25	van der Waals Interactions in Density-Functional Theory: Intermolecular Complexes. Journal of Chemical Theory and Computation, 2010, 6, 1081-1088.	2.3	155
26	Oscillations in meta-generalized-gradient approximation potential energy surfaces for dispersion-bound complexes. Journal of Chemical Physics, 2009, 131, 034111.	1.2	153
27	A density-functional approximation for relativistic kinetic energy. Journal of Chemical Physics, 2009, 131, 244118.	1.2	6
28	Van der Waals Interactions in Density-Functional Theory: Rare-Gas Diatomics. Journal of Chemical Theory and Computation, 2009, 5, 719-727.	2.3	145
29	Tests of an exact-exchange-based density-functional theory on transition-metal complexes. Canadian Journal of Chemistry, 2009, 87, 1369-1373.	0.6	24
30	A unified density-functional treatment of dynamical, nondynamical, and dispersion correlations. II. Thermochemical and kinetic benchmarks. Journal of Chemical Physics, 2008, 128, 124105.	1.2	39
31	Density functionals and transition-metal atoms. Journal of Chemical Physics, 2007, 126, 184104.	1.2	29
32	Exchange-hole dipole moment and the dispersion interaction revisited. Journal of Chemical Physics, 2007, 127, 154108.	1.2	432
33	A unified density-functional treatment of dynamical, nondynamical, and dispersion correlations. Journal of Chemical Physics, 2007, 127, 124108.	1.2	193
34	A post-Hartree-Fock model of intermolecular interactions: Inclusion of higher-order corrections. Journal of Chemical Physics, 2006, 124, 174104.	1.2	896
35	Exchange-hole dipole moment and the dispersion interaction: High-order dispersion coefficients. Journal of Chemical Physics, 2006, 124, 014104.	1.2	184
36	A simple effective potential for exchange. Journal of Chemical Physics, 2006, 124, 221101.	1.2	1,200

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37	Van der Waals interactions from the exchange hole dipole moment: Application to bio-organic benchmark systems. Chemical Physics Letters, 2006, 432, 600-603.	1.2	61
38	Exchange-hole dipole moment and the dispersion interaction. Journal of Chemical Physics, 2005, 122, 154104.	1.2	497
39	Real-space post-Hartreeâ€“Fock correlation models. Journal of Chemical Physics, 2005, 122, 064101.	1.2	231
40	A density-functional model of the dispersion interaction. Journal of Chemical Physics, 2005, 123, 154101.	1.2	1,150
41	A post-Hartreeâ€“Fock model of intermolecular interactions. Journal of Chemical Physics, 2005, 123, 024101.	1.2	735
42	A real-space model of nondynamical correlation. Journal of Chemical Physics, 2003, 119, 2972-2977.	1.2	200
43	Current density in exchange-correlation functionals: Application to atomic states. Journal of Chemical Physics, 2002, 117, 6935-6938.	1.2	102
44	Simulation of delocalized exchange by local density functionals. Journal of Chemical Physics, 2000, 112, 4020-4026.	1.2	165
45	Exploring the limits of gradient corrections in density functional theory. Journal of Computational Chemistry, 1999, 20, 63-69.	1.5	83
46	Optimized density functionals from the extended G2 test set. Journal of Chemical Physics, 1998, 108, 9624-9631.	1.2	694
47	Density-functional thermochemistry. V. Systematic optimization of exchange-correlation functionals. Journal of Chemical Physics, 1997, 107, 8554-8560.	1.2	1,673
48	Current-density dependent exchange-correlation functionals. Canadian Journal of Chemistry, 1996, 74, 995-997.	0.6	60
49	Local Density-Functional Polarizabilities and Hyperpolarizabilities at the Basis-Set Limit. The Journal of Physical Chemistry, 1996, 100, 16105-16108.	2.9	40
50	EXCHANGEâ€“CORRELATION APPROXIMATIONS IN DENSITY-FUNCTIONAL THEORY. Advanced Series in Physical Chemistry, 1995, , 1022-1046.	1.5	61
51	Thermochemical tests of a kinetic-energy dependent exchange-correlation approximation. International Journal of Quantum Chemistry, 1994, 52, 625-632.	1.0	81
52	Densityâ€functional thermochemistry. III. The role of exact exchange. Journal of Chemical Physics, 1993, 98, 5648-5652.	1.2	91,707
53	A new mixing of Hartreeâ€“Fock and local densityâ€functional theories. Journal of Chemical Physics, 1993, 98, 1372-1377.	1.2	14,273
54	Basis-set-free density-functional quantum chemistry. International Journal of Quantum Chemistry, 1989, 36, 599-609.	1.0	23