Aron J Cohen

List of Publications by Year
in descending order

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60 papers	19,383 citations	101384 36 h-index	128067 60 g-index
60 all docs	60 docs citations	60 times ranked	15688 citing authors

#	Article	IF	Citations
1	Revealing Noncovalent Interactions. Journal of the American Chemical Society, 2010, 132, 6498-6506.	6.6	6,465
2	Insights into Current Limitations of Density Functional Theory. Science, 2008, 321, 792-794.	6.0	2,057
3	Challenges for Density Functional Theory. Chemical Reviews, 2012, 112, 289-320.	23.0	1,869
4	Left-right correlation energy. Molecular Physics, 2001, 99, 403-412.	0.8	1,487
5	Development and assessment of new exchange-correlation functionals. Journal of Chemical Physics, 1998, 109, 6264-6271.	1.2	1,374
6	Localization and Delocalization Errors in Density Functional Theory and Implications for Band-Gap Prediction. Physical Review Letters, 2008, 100, 146401.	2.9	1,012
7	Many-electron self-interaction error in approximate density functionals. Journal of Chemical Physics, 2006, 125, 201102.	1.2	630
8	Fractional charge perspective on the band gap in density-functional theory. Physical Review B, 2008, 77, .	1.1	491
9	Assessment of a new local exchange functional OPTX. Chemical Physics Letters, 2001, 341, 319-328.	1.2	472
10	Dynamic correlation. Molecular Physics, 2001, 99, 607-615.	0.8	395
11	Development of exchange-correlation functionals with minimal many-electron self-interaction error. Journal of Chemical Physics, 2007, 126, 191109.	1.2	290
12	Fractional spins and static correlation error in density functional theory. Journal of Chemical Physics, 2008, 129, 121104.	1.2	215
13	Discontinuous Nature of the Exchange-Correlation Functional in Strongly Correlated Systems. Physical Review Letters, 2009, 102, 066403.	2.9	206
14	Self-interaction-free exchange-correlation functional for thermochemistry and kinetics. Journal of Chemical Physics, 2006, 124, 091102.	1.2	179
15	Pushing the frontiers of density functionals by solving the fractional electron problem. Science, 2021, 374, 1385-1389.	6.0	174
16	Improving Band Gap Prediction in Density Functional Theory from Molecules to Solids. Physical Review Letters, 2011, 107, 026403.	2.9	161
17	Delocalization errors in density functionals and implications for main-group thermochemistry. Journal of Chemical Physics, 2008, 129, 204112.	1.2	159
18	Derivative discontinuity, bandgap and lowest unoccupied molecular orbital in density functional theory. Journal of Chemical Physics, 2012, 136, 204111.	1.2	154

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19	Influence of Coulomb-attenuation on exchangeâ€“correlation functional quality. Physical Chemistry Chemical Physics, 2006, 8, 4543-4549.	1.3	127
20	Assessment of exchange correlation functionals. Chemical Physics Letters, 2000, 316, 160-166.	1.2	104
21	Evaluation of âŸ¨SÌ‚2âŸ© in density functional theory. Journal of Chemical Physics, 2007, 126, 214104.	1.2	97
22	Density functional calculations, using Slater basis sets, with exact exchange. Journal of Chemical Physics, 2003, 119, 6475-6481.	1.2	93
23	The derivative discontinuity of the exchangeâ€“correlation functional. Physical Chemistry Chemical Physics, 2014, 16, 14378-14387.	1.3	74
24	Local Scaling Correction for Reducing Delocalization Error in Density Functional Approximations. Physical Review Letters, 2015, 114, 053001.	2.9	69
25	Analytical evaluation of Fukui functions and real-space linear response function. Journal of Chemical Physics, 2012, 136, 144110.	1.2	67
26	Ab initio quantum mechanical/molecular mechanical simulation of electron transfer process: Fractional electron approach. Journal of Chemical Physics, 2008, 128, 124510.	1.2	61
27	Second-Order Perturbation Theory with Fractional Charges and Fractional Spins. Journal of Chemical Theory and Computation, 2009, 5, 786-792.	2.3	61
28	Thomasâ€“Fermiâ€“Diracâ€“von WeizsaÌˆcker models in finite systems. Journal of Chemical Physics, 2001, 114, 631.	1.2	59
29	Assessment and formal properties of exchange-correlation functionals constructed from the adiabatic connection. Journal of Chemical Physics, 2007, 127, 034101.	1.2	59
30	A dynamical correlation functional. Journal of Chemical Physics, 2002, 116, 5411-5418.	1.2	51
31	Failure of the random-phase-approximation correlation energy. Physical Review A, 2012, 85, .	1.0	51
32	Optimized effective potentials from electron densities in finite basis sets. Journal of Chemical Physics, 2007, 127, 174101.	1.2	48
33	Molecular electric properties: an assessment of recently developed functionals. Chemical Physics Letters, 1999, 299, 465-472.	1.2	47
34	Density functional calculations of the hyperpolarisabilities of small molecules. Chemical Physics Letters, 1999, 303, 391-398.	1.2	46
35	On the accuracy of density functional theory and wave function methods for calculating vertical ionization energies. Journal of Chemical Physics, 2015, 142, 194114.	1.2	44
36	Similarity transformation of the electronic SchrÃ¶dinger equation via Jastrow factorization. Journal of Chemical Physics, 2019, 151, 061101.	1.2	40

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37	A pseudobond parametrization for improved electrostatics in quantum mechanical/molecular mechanical simulations of enzymes. Journal of Chemical Physics, 2008, 129, 154106.	1.2	31
38	Extension of many-body theory and approximate density functionals to fractional charges and fractional spins. Journal of Chemical Physics, 2013, 139, 104114.	1.2	29
39	Density-functional generalized-gradient and hybrid calculations of electromagnetic properties using Slater basis sets. Journal of Chemical Physics, 2004, 120, 7252-7261.	1.2	28
40	Landscape of an exact energy functional. Physical Review A, 2016, 93, .	1.0	27
41	Dramatic changes in electronic structure revealed by fractionally charged nuclei. Journal of Chemical Physics, 2014, 140, 044110.	1.2	26
42	Calculation of nuclear magnetic resonance shielding constants using potential-based methods. Chemical Physics Letters, 2004, 399, 84-88.	1.2	25
43	Transition metal NMR chemical shifts from optimized effective potentials. Journal of Chemical Physics, 2007, 126, 074101.	1.2	22
44	Left-right and dynamic correlation. International Journal of Quantum Chemistry, 2002, 89, 86-93.	1.0	19
45	Excitation energies from time-dependent density functional theory with accurate exchange-correlation potentials. Molecular Physics, 2005, 103, 711-717.	0.8	19
46	Fermionic Statistics in the Strongly Correlated Limit of Density Functional Theory. Journal of Chemical Theory and Computation, 2017, 13, 6089-6100.	2.3	19
47	Density functional generalized gradient calculations using Slater basis sets. Journal of Chemical Physics, 2002, 117, 1470-1478.	1.2	18
48	Binding curve of the beryllium dimer using similarity-transformed FCIQMC: Spectroscopic accuracy with triple-zeta basis sets. Journal of Chemical Physics, 2021, 155, 011102.	1.2	18
49	Hartreeâ€“Fock orbitals which obey the nuclear cusp condition. Chemical Physics Letters, 2005, 404, 156-163.	1.2	17
50	Transcorrelated coupled cluster methods. Journal of Chemical Physics, 2021, 155, 191101.	1.2	17
51	Fractional numbers of electrons in Kohnâ€“Sham theory. Chemical Physics Letters, 2003, 382, 203-210.	1.2	13
52	Exact Density Functional Obtained via the Levy Constrained Search. Journal of Physical Chemistry Letters, 2018, 9, 4910-4914.	2.1	13
53	Analytic energy gradients of the optimized effective potential method. Journal of Chemical Physics, 2005, 123, 134111.	1.2	12
54	Are Hartreeâ€“Fock atoms too small or too large?. Physical Chemistry Chemical Physics, 2004, 6, 2928-2931.	1.3	9

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55	Qualitative breakdown of the unrestricted Hartree-Fock energy. Journal of Chemical Physics, 2014, 141, 164124.	1.2	9
56	Performance of a one-parameter correlation factor for transcorrelation: Study on a series of second row atomic and molecular systems. Journal of Chemical Physics, 2022, 156, .	1.2	8
57	Constructing a map from the electron density to the exchangeâ€“correlation potential. Physical Chemistry Chemical Physics, 2002, 4, 4612-4618.	1.3	5
58	Size extensivity of the direct optimized effective potential method. Journal of Chemical Physics, 2008, 128, 114702.	1.2	5
59	Optimized effective potential for calculations with orbital-free potential functionals. Molecular Physics, 2012, 110, 925-934.	0.8	3
60	Insight and progress in density functional theory. AIP Conference Proceedings, 2012, , .	0.3	3