Benjamin G Janesko

List of Publications by Year
in descending order

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113 papers	3,542 citations	159585 30 h-index	149698 56 g-index
115 all docs	115 docs citations	115 times ranked	4037 citing authors

#	Article	IF	Citations
1	Screened hybrid density functionals for solid-state chemistry and physics. Physical Chemistry Chemical Physics, 2009, 11, 443-454.	2.8	384
2	Generalized gradient approximation model exchange holes for range-separated hybrids. Journal of Chemical Physics, 2008, 128, 194105.	3.0	238
3	Observing Metal-Catalyzed Chemical Reactions in Situ Using Surface-Enhanced Raman Spectroscopy on Pdâ^'Au Nanoshells. Journal of the American Chemical Society, 2008, 130, 16592-16600.	13.7	185
4	Long-range-corrected hybrids including random phase approximation correlation. Journal of Chemical Physics, 2009, 130, 081105.	3.0	158
5	Hybrid functionals including random phase approximation correlation and second-order screened exchange. Journal of Chemical Physics, 2010, 132, 094103.	3.0	131
6	P(â•Ǒ)H to Pâ€“OH Tautomerism: A Theoretical and Experimental Study. Journal of Organic Chemistry, 2015, 80, 10025-10032.	3.2	114
7	Modeling interactions between lignocellulose and ionic liquids using DFT-D. Physical Chemistry Chemical Physics, 2011, 13, 11393.	2.8	112
8	Range Separation and Local Hybridization in Density Functional Theory. Journal of Physical Chemistry A, 2008, 112, 12530-12542.	2.5	94
9	Evaluation of range-separated hybrid density functionals for the prediction of vibrational frequencies, infrared intensities, and Raman activities. Physical Chemistry Chemical Physics, 2008, 10, 6621.	2.8	89
10	Hartreeâ€“Fock orbitals significantly improve the reaction barrier heights predicted by semilocal density functionals. Journal of Chemical Physics, 2008, 128, 244112.	3.0	89
11	Long-range-corrected hybrid density functionals including random phase approximation correlation: Application to noncovalent interactions. Journal of Chemical Physics, 2009, 131, 034110.	3.0	82
12	Replacing hybrid density functional theory: motivation and recent advances. Chemical Society Reviews, 2021, 50, 8470-8495.	38.1	80
13	Interactions of Ibuprofen with Hybrid Lipid Bilayers Probed by Complementary Surface-Enhanced Vibrational Spectroscopies. Journal of Physical Chemistry B, 2008, 112, 14168-14175.	2.6	70
14	Study of the Polydispersity of Grafted Poly(dimethylsiloxane) Surfaces Using Single-Molecule Atomic Force Microscopy. Journal of Physical Chemistry B, 2001, 105, 3965-3971.	2.6	68
15	Surface enhanced Raman optical activity of molecules on orientationally averaged substrates: Theory of electromagnetic effects. Journal of Chemical Physics, 2006, 125, 124704.	3.0	68
16	Self-consistent generalized Kohn-Sham local hybrid functionals of screened exchange: Combining local and range-separated hybridization. Journal of Chemical Physics, 2008, 129, 124110.	3.0	68
17	Chain-Length-Dependent Vibrational Resonances in Alkanethiol Self-Assembled Monolayers Observed on Plasmonic Nanoparticle Substrates. Nano Letters, 2006, 6, 2617-2621.	9.1	64
18	Acid-catalyzed hydrolysis of lignin Î²-O-4 linkages in ionic liquid solvents: a computational mechanistic study. Physical Chemistry Chemical Physics, 2014, 16, 5423.	2.8	55

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19	Local hybrid functionals based on density matrix products. Journal of Chemical Physics, 2007, 127, 164117.	3.0	54
20	Evaluation of Range-Separated Hybrid and Other Density Functional Approaches on Test Sets Relevant for Transition Metal-Based Homogeneous Catalysts. Journal of Physical Chemistry A, 2009, 113, 11742-11749.	2.5	50
21	Comparing modern density functionals for conjugated polymer band structures: Screened hybrid, Minnesota, and Rung 3.5 approximations. Journal of Chemical Physics, 2011, 134, 184105.	3.0	46
22	Parameterized local hybrid functionals from density-matrix similarity metrics. Journal of Chemical Physics, 2008, 128, 084111.	3.0	42
23	Using Catalytic and Surface-Enhanced Raman Spectroscopy-Active Gold Nanoshells to Understand the Role of Basicity in Glycerol Oxidation. ACS Catalysis, 2013, 3, 2430-2435.	11.2	40
24	Rung 3.5 density functionals. Journal of Chemical Physics, 2010, 133, 104103.	3.0	36
25	Practical Density Functionals beyond the Overdelocalizationâ€“Underbinding Zero-Sum Game. Journal of Physical Chemistry Letters, 2017, 8, 4314-4318.	4.6	35
26	Local hybrids as a perturbation to global hybrid functionals. Journal of Chemical Physics, 2009, 131, 154112.	3.0	33
27	How far do electrons delocalize?. Journal of Chemical Physics, 2014, 141, 144104.	3.0	32
28	pâ€Substituted Tris(2â€pyridylmethyl)amines as Ligands for Highly Active ATRP Catalysts: Facile Synthesis and Characterization. Angewandte Chemie - International Edition, 2020, 59, 14910-14920.	13.8	32
29	Comparative Study of Nonhybrid Density Functional Approximations for the Prediction of 3d Transition Metal Thermochemistry. Journal of Chemical Theory and Computation, 2017, 13, 4907-4913.	5.3	30
30	The role of the reference state in long-range random phase approximation correlation. Journal of Chemical Physics, 2009, 131, 154106.	3.0	29
31	Coulomb-only second-order perturbation theory in long-range-corrected hybrid density functionals. Physical Chemistry Chemical Physics, 2009, 11, 9677.	2.8	29
32	Rung 3.5 density functionals: Another step on Jacob's ladder. International Journal of Quantum Chemistry, 2013, 113, 83-88.	2.0	29
33	Locally rangeâ€separated hybrids as linear combinations of rangeâ€separated local hybrids. International Journal of Quantum Chemistry, 2009, 109, 2023-2032.	2.0	28
34	Role of the transition metal in Grignard metathesis polymerization (GRIM) of 3-hexylthiophene. Journal of Materials Chemistry A, 2013, 1, 12841.	10.3	27
35	Influence of the Alkyl Substituents Spacing on the Solar Cell Performance of Benzodithiophene Semiconducting Polymers. Macromolecules, 2012, 45, 772-780.	4.8	26
36	Unraveling the Role of Alkyl F on CHâ‹¯Ï€ Interactions and Uncovering the Tipping Point for Fluorophobicity. Journal of Organic Chemistry, 2015, 80, 7764-7769.	3.2	25

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37	When Hartree-Fock exchange admixture lowers DFT-predicted barrier heights: Natural bond orbital analyses and implications for catalysis. Journal of Chemical Physics, 2018, 148, 244106.	3.0	25
38	M11plus: A Range-Separated Hybrid Meta Functional with Both Local and Rung-3.5 Correlation Terms and High Across-the-Board Accuracy for Chemical Applications. Journal of Chemical Theory and Computation, 2019, 15, 4804-4815.	5.3	24
39	Practical auxiliary basis implementation of Rung 3.5 functionals. Journal of Chemical Physics, 2014, 141, 034103.	3.0	23
40	Using Constrained SchrÃ¶dinger Equations to Separate Resonant and Inductive Substituent Effects:Â A New Methodology for Parametrizing Simple Models in Chemistry. Journal of Physical Chemistry A, 2003, 107, 1655-1663.	2.5	22
41	Using Nonempirical Semilocal Density Functionals and Empirical Dispersion Corrections to Model Dative Bonding in Substituted Boranes. Journal of Chemical Theory and Computation, 2010, 6, 1825-1833.	5.3	22
42	Quantifying solvated electrons' delocalization. Physical Chemistry Chemical Physics, 2015, 17, 18305-18317.	2.8	22
43	An Orbital-Overlap Complement to Ligand and Binding Site Electrostatic Potential Maps. Journal of Chemical Information and Modeling, 2018, 58, 1836-1846.	5.4	22
44	Agostic Interactions in Nickel(II) Complexes: Trans Influence of Ancillary Ligands on the Strength of the Bond. Organometallics, 2014, 33, 84-93.	2.3	21
45	A simple nonlocal model for exchange. Journal of Chemical Physics, 2009, 131, 234111.	3.0	20
46	Nonspherical model density matrices for Rung 3.5 density functionals. Journal of Chemical Physics, 2012, 136, 024111.	3.0	20
47	Accurate Surface Chemistry beyond the Generalized Gradient Approximation: Illustrations for Graphene Adatoms. Journal of Chemical Theory and Computation, 2013, 9, 4853-4859.	5.3	20
48	Moleculeâ^'Surface Orientational Averaging in Surface Enhanced Raman Optical Activity Spectroscopy. Journal of Physical Chemistry C, 2009, 113, 9445-9449.	3.1	19
49	Triazine-Substituted and Acyl Hydrazones: Experiment and Computation Reveal a Stability Inversion at Low pH. Molecular Pharmaceutics, 2015, 12, 2924-2927.	4.6	19
50	Reducing density-driven error without exact exchange. Physical Chemistry Chemical Physics, 2017, 19, 4793-4801.	2.8	19
51	Long-range-corrected Rung 3.5 density functional approximations. Journal of Chemical Physics, 2018, 148, 104112.	3.0	18
52	Assessment of a density functional with full exact exchange and balanced non-locality of correlation. Molecular Physics, 2009, 107, 1077-1088.	1.7	17
53	Nonempirical Rung 3.5 density functionals from the Lieb-Oxford bound. Journal of Chemical Physics, 2012, 137, 224110.	3.0	17
54	Application of Screened Hybrid Density Functional Theory to Ammonia Decomposition on Silicon. Journal of Physical Chemistry C, 2012, 116, 26396-26404.	3.1	17

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55	Computational Investigation of Selectivity in Suzukiâ€“Miyaura Coupling of Secondary Alkyl Boranes. Organometallics, 2011, 30, 4564-4571.	2.3	15
56	A Benchmark Study of H₂ Activation by Au₃ and Ag₃ Clusters. Journal of Physical Chemistry C, 2013, 117, 7487-7496.	3.1	15
57	3-Methyleneisoindolin-1-one Assembly via Base- and CuI/<scp>l</scp>-Proline-Catalyzed Domino Reaction: Mechanism of Regioselective Anionic Cyclization. Journal of Organic Chemistry, 2016, 81, 10802-10808.	3.2	15
58	Quantifying Electron Delocalization in Electrides. Journal of Chemical Theory and Computation, 2016, 12, 79-91.	5.3	15
59	Magnetic exchange couplings evaluated with Rung 3.5 density functionals. Journal of Chemical Physics, 2011, 134, 214101.	3.0	14
60	Computational Mechanistic Study of Stereoselective Suzuki Coupling of an Î±-Cyano-Activated Secondary Alkyl. Organometallics, 2012, 31, 4610-4618.	2.3	13
61	Evaluation of Approximate Exchange-Correlation Functionals in Predicting One-Bond ³¹Pâ€“¹H NMR Indirect Spinâ€“Spin Coupling Constants. Journal of Chemical Theory and Computation, 2013, 9, 1443-1451.	5.3	13
62	Using molecular similarity to construct accurate semiempirical electronic structure theories. Journal of Chemical Physics, 2004, 121, 5635-5645.	3.0	11
63	Synthesis, characterization, and computational modeling of benzodithiophene donorâ€“acceptor semiconducting polymers. Journal of Polymer Science Part A, 2011, 49, 4172-4179.	2.3	11
64	Electron Delocalization Range in Atoms and on Molecular Surfaces. Journal of Chemical Theory and Computation, 2016, 12, 3185-3194.	5.3	11
65	Quantum Chemical Fragment Precursor Tests: Accelerating de novo annotation of tandem mass spectra. Analytica Chimica Acta, 2017, 995, 52-64.	5.4	11
66	Why are GGAs so accurate for reaction kinetics on surfaces? Systematic comparison of hybrid vs. nonhybrid DFT for representative reactions. Journal of Chemical Physics, 2017, 146, 234103.	3.0	11
67	M11plus, a Range-Separated Hybrid Meta Functional Incorporating Nonlocal Rung-3.5 Correlation, Exhibits Broad Accuracy on Diverse Databases. Journal of Physical Chemistry Letters, 2020, 11, 3045-3050.	4.6	10
68	Explicitly correlated divide-and-conquer-type electronic structure calculations based on two-electron reduced density matrices. Journal of Chemical Physics, 2003, 119, 1320-1328.	3.0	9
69	Density Functional Theory Beyond the Generalized Gradient Approximation for Surface Chemistry. Topics in Current Chemistry, 2014, , 25-51.	4.0	9
70	Tunable Fictitious Substituent Effects on the Ï€â€“Ï€ Interactions of Substituted Sandwich Benzene Dimers. Journal of Physical Chemistry A, 2014, 118, 3344-3350.	2.5	9
71	Simulating Goldâ€™s Structure-Dependent Reactivity: Nonlocal Density Functional Theory Studies of Hydrogen Activation by Gold Clusters, Nanowires, and Surfaces. Journal of Physical Chemistry C, 2014, 118, 15693-15704.	3.1	9
72	Topological analysis of the electron delocalization range. Journal of Computational Chemistry, 2016, 37, 1993-2005.	3.3	9

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73	Performance of new density functionals of nondynamic correlation on chemical properties. Journal of Chemical Physics, 2019, 150, 204101.	3.0	9
74	Quantifying the delocalization of surface and bulk F-centers. Surface Science, 2017, 659, 9-15.	1.9	8
75	An Orbitalâ€Overlap Complement to Atomic Partial Charge. Angewandte Chemie - International Edition, 2017, 56, 6878-6881.	13.8	8
76	A new triazine bearing a pyrazolone group capable of copper, nickel, and zinc chelation. RSC Advances, 2018, 8, 3024-3035.	3.6	8
77	Density functionals for nondynamical correlation constructed from an upper bound to the exact exchange energy density. Molecular Physics, 2019, 117, 1226-1241.	1.7	8
78	Mechanistic Insights into Iron-Catalyzed Câ€“H Bond Activation and Câ€“C Coupling. Organometallics, 2021, 40, 2467-2477.	2.3	8
79	Efficient syntheses of macrocycles ranging from 22â€“28 atoms through spontaneous dimerization to yield bis-hydrazones. RSC Advances, 2020, 10, 3217-3220.	3.6	7
80	The electron delocalization range in stretched bonds. International Journal of Quantum Chemistry, 2016, 116, 1783-1795.	2.0	6
81	Synthesis of Macrocycles Derived from Substituted Triazines. ChemBioChem, 2019, 20, 241-246.	2.6	6
82	Virtual Experiments on Real Asphaltenes: Predicting Properties Using Quantum Chemical Simulations of Structures from Non-contact Atomic Force Microscopy. Energy & Fuels, 2022, 36, 8714-8724.	5.1	6
83	Left-right correlation in coupled F-center defects. Journal of Chemical Physics, 2016, 145, 054703.	3.0	5
84	Accurate alkynyl radical structures from density functional calculations without Hartree-Fock exchange. Journal of Chemical Physics, 2017, 146, 054109.	3.0	5
85	Computational study of fluoroquinolone binding to Mg(H2O)N2+ and its applicability to future drug design. International Journal of Quantum Chemistry, 2017, 117, e25428.	2.0	5
86	Delocalization Error in DFT-Predicted Extreme Long-Range Functionalization of Carbon-Doped Hexagonal Boron Nitride. Journal of Physical Chemistry C, 2019, 123, 15062-15070.	3.1	5
87	Half-Pancake Bonding in Asphaltenes. Energy & Fuels, 0, , .	5.1	5
88	Adiabatic projection: Bridging ab initio, density functional, semiempirical, and embedding approximations. Journal of Chemical Physics, 2022, 156, 014111.	3.0	5
89	Systematically Improvable Generalization of Self-Interaction Corrected Density Functional Theory. Journal of Physical Chemistry Letters, 2022, 13, 5698-5702.	4.6	5
90	Frustrated Lewis Pair Nanoribbons. Journal of Physical Chemistry C, 2012, 116, 16467-16472.	3.1	4

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91	Strong correlation in surface chemistry. Molecular Simulation, 2017, 43, 394-405.	2.0	4
92	Attractive Nonbonded Interactions Help Stabilize the Z Form of Alkenyl Anions. Journal of Organic Chemistry, 2018, 83, 8208-8213.	3.2	4
93	Functional Group Basis Sets. Journal of Chemical Theory and Computation, 2005, 1, 267-278.	5.3	3
94	Dispersion-corrected DFT study of methano and ethano bridged Wilcox torsion balances. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	3
95	Ligand effects on the redox behavior of bimetallic tungsten(0)/ferrocene(II) complexes. Polyhedron, 2014, 72, 50-55.	2.2	3
96	Simulating periodic trends in the structure and catalytic activity of coinage metal nanoribbons. International Journal of Quantum Chemistry, 2015, 115, 1718-1725.	2.0	3
97	Testing Exact Upper Bounds to Exact Exchange. Journal of Chemical Theory and Computation, 2017, 13, 1980-1988.	5.3	3
98	Time-dependent broken-symmetry density functional theory simulation of the optical response of entangled paramagnetic defects: Color centers in lithium fluoride. Physical Review B, 2018, 97, .	3.2	3
99	Nonlocal rung-3.5 correlation from the density matrix expansion: Flat-plane condition, thermochemistry, and kinetics. Journal of Chemical Physics, 2020, 153, 164116.	3.0	3
100	Revisiting alternative pathways in the Fischerâ€“Tropsch process: Accurate density functional theory calculations on â€œmagicâ€•Ru₁₂ clusters. International Journal of Quantum Chemistry, 2016, 116, 1451-1458.	2.0	2
101	Predicting ion mobility collision cross sections directly from standard quantum chemistry software. Journal of Mass Spectrometry, 2018, 53, 432-434.	1.6	2
102	Density functionals with full nonlocal exchange, nonlocal rungâ€3.5 correlation, and <scp>D3</scp> dispersion: Combined accuracy for general mainâ€group thermochemistry, kinetics, and noncovalent interactions. Journal of Computational Chemistry, 2021, 42, 1974-1981.	3.3	2
103	Extending the Marcus Î¼-Scale of Solvent Softness Using Conceptual Density Functional Theory and the Orbital Overlap Distance: Method and Application to Ionic Liquids. Journal of Solution Chemistry, 2020, 49, 614-628.	1.2	2
104	Dispersion-corrected Rung 3.5 density functionals. Theoretical Chemistry Accounts, 2013, 132, 1.	1.4	1
105	Modeling continuous changes in substituent electronegativity and chemical hardness using fictitious nuclear potentials. Theoretical Chemistry Accounts, 2013, 132, 1.	1.4	1
106	Calculation of magnetic properties with density functional approximations including rung 3.5 ingredients. Journal of Chemical Physics, 2020, 153, 164101.	3.0	1
107	Benchmarking timeâ€dependent density functional theory predictions of emission spectra and <scp>CIE</scp> color: A rainbow of error. International Journal of Quantum Chemistry, 0, , .	2.0	1
108	Chain-Length-Dependent Vibrational Resonances in Alkanethiol Self-Assembled Monolayers Observed on Plasmonic Nanoparticle Substrates. Nano Letters, 2007, 7, 853-853.	9.1	0

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109	An Orbitalâ€Overlap Complement to Atomic Partial Charge. Angewandte Chemie, 2017, 129, 6982-6985.	2.0	0
110	TEMPORARY REMOVAL: A hydrogen bond and strong electron withdrawing group lead to the formation of surprisingly stable, cyclic hemiaminals. Tetrahedron Letters, 2019, , 151334.	1.4	0
111	Coupled alkali halide color centers: Fractional charge errors, fractional spin errors, and a failure of spin symmetry breaking produce challenging tests for condensed-phase electronic structure calculations. Journal of Chemical Physics, 2019, 151, 064109.	3.0	0
112	Tunable model promoters in DFT simulations of catalysts. Journal of Computational Chemistry, 2019, 40, 1752-1757.	3.3	0
113	Density Functional Theory for Transition Metal Catalysis. , 2024, , 562-585.		0