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	Density Functional Theory for Transition Metal Catalysis. , 2024, , 562-585.		0
2	Adiabatic projection: Bridging ab initio, density functional, semiempirical, and embedding approximations. Journal of Chemical Physics, 2022, 156, 014111.	3.0	5
3	Systematically Improvable Generalization of Self-Interaction Corrected Density Functional Theory. Journal of Physical Chemistry Letters, 2022, 13, 5698-5702.	4.6	5
4	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
5	Replacing hybrid density functional theory: motivation and recent advances. Chemical Society Reviews, 2021, 50, 8470-8495.	38.1	80
6	Mechanistic Insights into Iron-Catalyzed Câ€“H Bond Activation and Câ€“C Coupling. Organometallics, 2021, 40, 2467-2477.	2.3	8
7	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
8	Calculation of magnetic properties with density functional approximations including rung 3.5 ingredients. Journal of Chemical Physics, 2020, 153, 164101.	3.0	1
9	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
10	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
11	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
12	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
13	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
14	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
15	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
16	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
17	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
18	Performance of new density functionals of nondynamic correlation on chemical properties. Journal of Chemical Physics, 2019, 150, 204101.	3.0	9

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19	Tunable model promoters in DFT simulations of catalysts. Journal of Computational Chemistry, 2019, 40, 1752-1757.	3.3	0
20	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
21	Synthesis of Macrocycles Derived from Substituted Triazines. ChemBioChem, 2019, 20, 241-246.	2.6	6
22	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
23	Predicting ion mobility collision cross sections directly from standard quantum chemistry software. Journal of Mass Spectrometry, 2018, 53, 432-434.	1.6	2
24	Long-range-corrected Rung 3.5 density functional approximations. Journal of Chemical Physics, 2018, 148, 104112.	3.0	18
25	A new triazine bearing a pyrazolone group capable of copper, nickel, and zinc chelation. RSC Advances, 2018, 8, 3024-3035.	3.6	8
26	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
27	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
28	Attractive Nonbonded Interactions Help Stabilize the Z Form of Alkenyl Anions. Journal of Organic Chemistry, 2018, 83, 8208-8213.	3.2	4
29	Reducing density-driven error without exact exchange. Physical Chemistry Chemical Physics, 2017, 19, 4793-4801.	2.8	19
30	Quantifying the delocalization of surface and bulk F-centers. Surface Science, 2017, 659, 9-15.	1.9	8
31	Strong correlation in surface chemistry. Molecular Simulation, 2017, 43, 394-405.	2.0	4
32	Accurate alkynyl radical structures from density functional calculations without Hartree-Fock exchange. Journal of Chemical Physics, 2017, 146, 054109.	3.0	5
33	An Orbitalâ€Overlap Complement to Atomic Partial Charge. Angewandte Chemie - International Edition, 2017, 56, 6878-6881.	13.8	8
34	An Orbitalâ€Overlap Complement to Atomic Partial Charge. Angewandte Chemie, 2017, 129, 6982-6985.	2.0	0
35	Testing Exact Upper Bounds to Exact Exchange. Journal of Chemical Theory and Computation, 2017, 13, 1980-1988.	5.3	3
36	Quantum Chemical Fragment Precursor Tests: Accelerating de novo annotation of tandem mass spectra. Analytica Chimica Acta, 2017, 995, 52-64.	5.4	11

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37	Practical Density Functionals beyond the Overdelocalizationâ€“Underbinding Zero-Sum Game. Journal of Physical Chemistry Letters, 2017, 8, 4314-4318.	4.6	35
38	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
39	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
40	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
41	Topological analysis of the electron delocalization range. Journal of Computational Chemistry, 2016, 37, 1993-2005.	3.3	9
42	Left-right correlation in coupled F-center defects. Journal of Chemical Physics, 2016, 145, 054703.	3.0	5
43	The electron delocalization range in stretched bonds. International Journal of Quantum Chemistry, 2016, 116, 1783-1795.	2.0	6
44	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
45	3-Methyleneisoindolin-1-one Assembly via Base- and CuI/<scp>I</scp>-Proline-Catalyzed Domino Reaction: Mechanism of Regioselective Anionic Cyclization. Journal of Organic Chemistry, 2016, 81, 10802-10808.	3.2	15
46	Electron Delocalization Range in Atoms and on Molecular Surfaces. Journal of Chemical Theory and Computation, 2016, 12, 3185-3194.	5.3	11
47	Quantifying Electron Delocalization in Electrides. Journal of Chemical Theory and Computation, 2016, 12, 79-91.	5.3	15
48	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
49	Quantifying solvated electrons' delocalization. Physical Chemistry Chemical Physics, 2015, 17, 18305-18317.	2.8	22
50	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
51	Triazine-Substituted and Acyl Hydrazones: Experiment and Computation Reveal a Stability Inversion at Low pH. Molecular Pharmaceutics, 2015, 12, 2924-2927.	4.6	19
52	P(â•O)H to Pâ€“OH Tautomerism: A Theoretical and Experimental Study. Journal of Organic Chemistry, 2015, 80, 10025-10032.	3.2	114
53	Practical auxiliary basis implementation of Rung 3.5 functionals. Journal of Chemical Physics, 2014, 141, 034103.	3.0	23
54	How far do electrons delocalize?. Journal of Chemical Physics, 2014, 141, 144104.	3.0	32

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55	Density Functional Theory Beyond the Generalized Gradient Approximation for Surface Chemistry. Topics in Current Chemistry, 2014, , 25-51.	4.0	9
56	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
57	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
58	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
59	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
60	Dispersion-corrected DFT study of methano and ethano bridged Wilcox torsion balances. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	3
61	Ligand effects on the redox behavior of bimetallic tungsten(0)/ferrocene(II) complexes. Polyhedron, 2014, 72, 50-55.	2.2	3
62	Rung 3.5 density functionals: Another step on Jacob's ladder. International Journal of Quantum Chemistry, 2013, 113, 83-88.	2.0	29
63	Dispersion-corrected Rung 3.5 density functionals. Theoretical Chemistry Accounts, 2013, 132, 1.	1.4	1
64	Role of the transition metal in Grignard metathesis polymerization (GRIM) of 3-hexylthiophene. Journal of Materials Chemistry A, 2013, 1, 12841.	10.3	27
65	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
66	Modeling continuous changes in substituent electronegativity and chemical hardness using fictitious nuclear potentials. Theoretical Chemistry Accounts, 2013, 132, 1.	1.4	1
67	A Benchmark Study of H₂ Activation by Au₃ and Ag₃ Clusters. Journal of Physical Chemistry C, 2013, 117, 7487-7496.	3.1	15
68	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
69	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
70	Nonspherical model density matrices for Rung 3.5 density functionals. Journal of Chemical Physics, 2012, 136, 024111.	3.0	20
71	Nonempirical Rung 3.5 density functionals from the Lieb-Oxford bound. Journal of Chemical Physics, 2012, 137, 224110.	3.0	17
72	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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73	Influence of the Alkyl Substituents Spacing on the Solar Cell Performance of Benzodithiophene Semiconducting Polymers. Macromolecules, 2012, 45, 772-780.	4.8	26
74	Frustrated Lewis Pair Nanoribbons. Journal of Physical Chemistry C, 2012, 116, 16467-16472.	3.1	4
75	Computational Mechanistic Study of Stereoselective Suzuki Coupling of an Î±-Cyano-Activated Secondary Alkyl. Organometallics, 2012, 31, 4610-4618.	2.3	13
76	Modeling interactions between lignocellulose and ionic liquids using DFT-D. Physical Chemistry Chemical Physics, 2011, 13, 11393.	2.8	112
77	Computational Investigation of Selectivity in Suzukiâ€“Miyaura Coupling of Secondary Alkyl Boranes. Organometallics, 2011, 30, 4564-4571.	2.3	15
78	Magnetic exchange couplings evaluated with Rung 3.5 density functionals. Journal of Chemical Physics, 2011, 134, 214101.	3.0	14
79	Synthesis, characterization, and computational modeling of benzodithiophene donorâ€“acceptor semiconducting polymers. Journal of Polymer Science Part A, 2011, 49, 4172-4179.	2.3	11
80	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
81	Hybrid functionals including random phase approximation correlation and second-order screened exchange. Journal of Chemical Physics, 2010, 132, 094103.	3.0	131
82	Rung 3.5 density functionals. Journal of Chemical Physics, 2010, 133, 104103.	3.0	36
83	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
84	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
85	Local hybrids as a perturbation to global hybrid functionals. Journal of Chemical Physics, 2009, 131, 154112.	3.0	33
86	The role of the reference state in long-range random phase approximation correlation. Journal of Chemical Physics, 2009, 131, 154106.	3.0	29
87	Locally rangeâ€separated hybrids as linear combinations of rangeâ€separated local hybrids. International Journal of Quantum Chemistry, 2009, 109, 2023-2032.	2.0	28
88	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
89	Coulomb-only second-order perturbation theory in long-range-corrected hybrid density functionals. Physical Chemistry Chemical Physics, 2009, 11, 9677.	2.8	29
90	Moleculeâ^'Surface Orientational Averaging in Surface Enhanced Raman Optical Activity Spectroscopy. Journal of Physical Chemistry C, 2009, 113, 9445-9449.	3.1	19

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91	Long-range-corrected hybrids including random phase approximation correlation. Journal of Chemical Physics, 2009, 130, 081105.	3.0	158
92	Screened hybrid density functionals for solid-state chemistry and physics. Physical Chemistry Chemical Physics, 2009, 11, 443-454.	2.8	384
93	Assessment of a density functional with full exact exchange and balanced non-locality of correlation. Molecular Physics, 2009, 107, 1077-1088.	1.7	17
94	A simple nonlocal model for exchange. Journal of Chemical Physics, 2009, 131, 234111.	3.0	20
95	Generalized gradient approximation model exchange holes for range-separated hybrids. Journal of Chemical Physics, 2008, 128, 194105.	3.0	238
96	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
97	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
98	Range Separation and Local Hybridization in Density Functional Theory. Journal of Physical Chemistry A, 2008, 112, 12530-12542.	2.5	94
99	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
100	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
101	Hartreeâ€"Fock orbitals significantly improve the reaction barrier heights predicted by semilocal density functionals. Journal of Chemical Physics, 2008, 128, 244112.	3.0	89
102	Parameterized local hybrid functionals from density-matrix similarity metrics. Journal of Chemical Physics, 2008, 128, 084111.	3.0	42
103	Local hybrid functionals based on density matrix products. Journal of Chemical Physics, 2007, 127, 164117.	3.0	54
104	Chain-Length-Dependent Vibrational Resonances in Alkanethiol Self-Assembled Monolayers Observed on Plasmonic Nanoparticle Substrates. Nano Letters, 2007, 7, 853-853.	9.1	0
105	Chain-Length-Dependent Vibrational Resonances in Alkanethiol Self-Assembled Monolayers Observed on Plasmonic Nanoparticle Substrates. Nano Letters, 2006, 6, 2617-2621.	9.1	64
106	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
107	Functional Group Basis Sets. Journal of Chemical Theory and Computation, 2005, 1, 267-278.	5.3	3
108	Using molecular similarity to construct accurate semiempirical electronic structure theories. Journal of Chemical Physics, 2004, 121, 5635-5645.	3.0	11

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109	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
110	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
111	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
112	Half-Pancake Bonding in Asphaltenes. Energy & Fuels, 0, , .	5.1	5
113	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