Neil Qiang Su

List of Publications by Year
in descending order

48 papers	1,802 citations	331670 21 h-index	265206 42 g-index
49 all docs	49 docs citations	49 times ranked	1992 citing authors

#	Article	IF	Citations
1	Product selectivity in plasmonic photocatalysis for carbon dioxide hydrogenation. Nature Communications, 2017, 8, 14542.	12.8	348
2	Plasmon-Enhanced Catalysis: Distinguishing Thermal and Nonthermal Effects. Nano Letters, 2018, 18, 1714-1723.	9.1	251
3	Benchmarking Density Functionals on Structural Parameters of Small-/Medium-Sized Organic Molecules. Journal of Chemical Theory and Computation, 2016, 12, 459-465.	5.3	165
4	Localized orbital scaling correction for systematic elimination of delocalization error in density functional approximations. National Science Review, 2018, 5, 203-215.	9.5	110
5	Doubly hybrid density functional xDH-PBE0 from a parameter-free global hybrid model PBE0. Journal of Chemical Physics, 2012, 136, 174103.	3.0	99
6	Construction of a parameter-free doubly hybrid density functional from adiabatic connection. Journal of Chemical Physics, 2014, 140, 18A512.	3.0	57
7	Describing strong correlation with fractional-spin correction in density functional theory. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 9678-9683.	7.1	56
8	The <scp>XYG3</scp> type of doubly hybrid density functionals. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2016, 6, 721-747.	14.6	52
9	Development of New Density Functional Approximations. Annual Review of Physical Chemistry, 2017, 68, 155-182.	10.8	51
10	Fractional Charge Behavior and Band Gap Predictions with the XYG3 Type of Doubly Hybrid Density Functionals. Journal of Physical Chemistry A, 2014, 118, 9201-9211.	2.5	45
11	Beyond Mean-Field Microkinetics: Toward Accurate and Efficient Theoretical Modeling in Heterogeneous Catalysis. ACS Catalysis, 2018, 8, 5816-5826.	11.2	41
12	Doubly hybrid density functionals that correctly describe both density and energy for atoms. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 2287-2292.	7.1	36
13	A comparison of geometric parameters from PBE-based doubly hybrid density functionals PBE0-DH, PBE0-2, and xDH-PBE0. Journal of Chemical Physics, 2013, 139, 174106.	3.0	32
14	Describing Chemical Reactivity with Frontier Molecular Orbitalets. Jacs Au, 2022, 2, 1383-1394.	7.9	32
15	Preserving Symmetry and Degeneracy in the Localized Orbital Scaling Correction Approach. Journal of Physical Chemistry Letters, 2020, 11, 1528-1535.	4.6	31
16	Analytic derivatives for the XYG3 type of doubly hybrid density functionals: Theory, implementation, and assessment. Journal of Computational Chemistry, 2013, 34, 1759-1774.	3.3	26
17	Approximating Quasiparticle and Excitation Energies from Ground State Generalized Kohnâ€“Sham Calculations. Journal of Physical Chemistry A, 2019, 123, 666-673.	2.5	26
18	Calculations of ionization energies and electron affinities for atoms and molecules: A comparative study with different methods. Frontiers of Chemistry in China: Selected Publications From Chinese Universities, 2011, 6, 269-279.	0.4	22

#	Article	IF	Citations
19	Toward the construction of parameterâ€free doubly hybrid density functionals. International Journal of Quantum Chemistry, 2015, 115, 589-595.	2.0	22
20	Double Hybrid Functionals and the Î-System Bond Length Alternation Challenge: Rivaling Accuracy of Post-HF Methods. Journal of Chemical Theory and Computation, 2015, 11, 832-838.	5.3	22
21	Computational Insight into Metallated Graphynes as Single Atom Electrocatalysts for Nitrogen Fixation. ACS Applied Materials & Interfaces, 2022, 14, 27861-27872.	8.0	22
22	Multireference Density Functional Theory with Generalized Auxiliary Systems for Ground and Excited States. Journal of Physical Chemistry Letters, 2017, 8, 4479-4485.	4.6	21
23	Beyond energies: geometry predictions with the XYG3 type of doubly hybrid density functionals. Chemical Communications, 2016, 52, 13840-13860.	4.1	18
24	Generalized Optimized Effective Potential for Orbital Functionals and Self-Consistent Calculation of Random Phase Approximations. Journal of Physical Chemistry Letters, 2017, 8, 4746-4751.	4.6	18
25	Accurate Quasiparticle Spectra from the T-Matrix Self-Energy and the Particleâ€“Particle Random Phase Approximation. Journal of Physical Chemistry Letters, 2017, 8, 3223-3227.	4.6	18
26	Renormalized Singles Greenâ€™s Function for Quasi-Particle Calculations beyond the G₀W₀ Approximation. Journal of Physical Chemistry Letters, 2019, 10, 447-452.	4.6	17
27	Insights into Direct Methods for Predictions of Ionization Potential and Electron Affinity in Density Functional Theory. Journal of Physical Chemistry Letters, 2019, 10, 2692-2699.	4.6	16
28	Integration Approach at the Second-Order Perturbation Theory: Applications to Ionization Potential and Electron Affinity Calculations. Journal of Chemical Theory and Computation, 2015, 11, 4677-4688.	5.3	14
29	Second-Order Perturbation Theory for Fractional Occupation Systems: Applications to Ionization Potential and Electron Affinity Calculations. Journal of Chemical Theory and Computation, 2016, 12, 2285-2297.	5.3	14
30	Error Accumulations in Adhesive Energies of Dihydrogen Molecular Chains: Performances of the XYG3 Type of Doubly Hybrid Density Functionals. Journal of Physical Chemistry A, 2015, 119, 1590-1599.	2.5	13
31	H + H2 quantum dynamics using potential energy surfaces based on the XYG3 type of doubly hybrid density functionals: Validation of the density functionals. Journal of Chemical Physics, 2015, 142, 084107.	3.0	11
32	Unity of Kohn-Sham density-functional theory and reduced-density-matrix-functional theory. Physical Review A, 2021, 104, .	2.5	11
33	A comparative study of the xDH-PBE0 and DSD-PBEPBE-D3BJ doubly hybrid density functionals. Molecular Physics, 2016, 114, 1207-1217.	1.7	10
34	Handling Ensemble N-Representability Constraint in Explicit-by-Implicit Manner. Journal of Physical Chemistry Letters, 2021, 12, 6788-6793.	4.6	10
35	Response to â€œComment on â€˜Doubly hybrid density functional xDH-PBE0 from a parameter-free global hybrid model PBE0â€â€™ [J. Chem. Phys. 143, 187101 (2015)]. Journal of Chemical Physics, 2015, 143, 187102.	3.0	8
36	LibSC: Library for Scaling Correction Methods in Density Functional Theory. Journal of Chemical Theory and Computation, 2022, 18, 840-850.	5.3	8

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37	The Role of Range-Separated Correlation in Long-Range Corrected Hybrid Functionals. Journal of Physical Chemistry Letters, 2021, 12, 1207-1213.	4.6	7
38	Introductory lecture: when the density of the noninteracting reference system is not the density of the physical system in density functional theory. Faraday Discussions, 2020, 224, 9-26.	3.2	6
39	Functional-Based Description of Electronic Dynamic and Strong Correlation: Old Issues and New Insights. Journal of Physical Chemistry Letters, 2022, 13, 1744-1751.	4.6	6
40	Combining Localized Orbital Scaling Correction and Bethe-Salpeter Equation for Accurate Excitation Energies. Journal of Chemical Physics, 2022, 156, 154101.	3.0	6
41	When does a functional correctly describe both the structure and the energy of the transition state?. Journal of Molecular Modeling, 2017, 23, 65.	1.8	5
42	Revisiting the Hole Size in Double Helical DNA with Localized Orbital Scaling Corrections. Journal of Physical Chemistry B, 2020, 124, 3428-3435.	2.6	5
43	Accurate potential energy surfaces for hydrogen abstraction reactions: A benchmark study on the XYG3 doubly hybrid density functional. Journal of Computational Chemistry, 2017, 38, 2326-2334.	3.3	4
44	Recent progress of the XYG3 type of doubly hybrid functionals: From energy calculations to analytic geometry optimizations. Scientia Sinica Chimica, 2013, 43, 1761-1779.	0.4	3
45	Approximate functionals in hypercomplex Kohnâ€“Sham theory. Electronic Structure, 2022, 4, 014011.	2.8	3
46	Self-consistent field for fragmented quantum mechanical model of large molecular systems. Journal of Computational Chemistry, 2016, 37, 321-326.	3.3	2
47	Perturbative treatment of anharmonic vibrational effects on bond distances: An extended langevin dynamics method. Journal of Computational Chemistry, 2014, 35, 467-478.	3.3	1
48	Perturbation theory made efficient and effective for predictions of ionization potential and electron affinity. Journal of Chemical Physics, 2021, 154, 174101.	3.0	1