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	LibSC: Library for Scaling Correction Methods in Density Functional Theory. Journal of Chemical Theory and Computation, 2022, 18, 840-850.	5.3	8
2	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
3	Approximate functionals in hypercomplex Kohnâ€“Sham theory. Electronic Structure, 2022, 4, 014011.	2.8	3
4	Combining Localized Orbital Scaling Correction and Bethe-Salpeter Equation for Accurate Excitation Energies. Journal of Chemical Physics, 2022, 156, 154101.	3.0	6
5	Computational Insight into Metallated Graphynes as Single Atom Electrocatalysts for Nitrogen Fixation. ACS Applied Materials & Interfaces, 2022, 14, 27861-27872.	8.0	22
6	Describing Chemical Reactivity with Frontier Molecular Orbitalets. Jacs Au, 2022, 2, 1383-1394.	7.9	32
7	The Role of Range-Separated Correlation in Long-Range Corrected Hybrid Functionals. Journal of Physical Chemistry Letters, 2021, 12, 1207-1213.	4.6	7
8	Perturbation theory made efficient and effective for predictions of ionization potential and electron affinity. Journal of Chemical Physics, 2021, 154, 174101.	3.0	1
9	Handling Ensemble N-Representability Constraint in Explicit-by-Implicit Manner. Journal of Physical Chemistry Letters, 2021, 12, 6788-6793.	4.6	10
10	Unity of Kohn-Sham density-functional theory and reduced-density-matrix-functional theory. Physical Review A, 2021, 104, .	2.5	11
11	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
12	Preserving Symmetry and Degeneracy in the Localized Orbital Scaling Correction Approach. Journal of Physical Chemistry Letters, 2020, 11, 1528-1535.	4.6	31
13	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
14	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
15	Approximating Quasiparticle and Excitation Energies from Ground State Generalized Kohnâ€“Sham Calculations. Journal of Physical Chemistry A, 2019, 123, 666-673.	2.5	26
16	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
17	Beyond Mean-Field Microkinetics: Toward Accurate and Efficient Theoretical Modeling in Heterogeneous Catalysis. ACS Catalysis, 2018, 8, 5816-5826.	11.2	41
18	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

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19	Plasmon-Enhanced Catalysis: Distinguishing Thermal and Nonthermal Effects. Nano Letters, 2018, 18, 1714-1723.	9.1	251
20	Localized orbital scaling correction for systematic elimination of delocalization error in density functional approximations. National Science Review, 2018, 5, 203-215.	9.5	110
21	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
22	Product selectivity in plasmonic photocatalysis for carbon dioxide hydrogenation. Nature Communications, 2017, 8, 14542.	12.8	348
23	Development of New Density Functional Approximations. Annual Review of Physical Chemistry, 2017, 68, 155-182.	10.8	51
24	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
25	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
26	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
27	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
28	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
29	Self-consistent field for fragmented quantum mechanical model of large molecular systems. Journal of Computational Chemistry, 2016, 37, 321-326.	3.3	2
30	Beyond energies: geometry predictions with the XYG3 type of doubly hybrid density functionals. Chemical Communications, 2016, 52, 13840-13860.	4.1	18
31	The <scp>XYG3</scp> type of doubly hybrid density functionals. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2016, 6, 721-747.	14.6	52
32	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
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	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
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	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

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37	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
38	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
39	Toward the construction of parameterâ€free doubly hybrid density functionals. International Journal of Quantum Chemistry, 2015, 115, 589-595.	2.0	22
40	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
41	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
42	Construction of a parameter-free doubly hybrid density functional from adiabatic connection. Journal of Chemical Physics, 2014, 140, 18A512.	3.0	57
43	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
44	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
45	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
46	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
47	Doubly hybrid density functional xDH-PBE0 from a parameter-free global hybrid model PBE0. Journal of Chemical Physics, 2012, 136, 174103.	3.0	99
48	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