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List of Publications by Year
in descending order

26 papers	1,017 citations	623734 14 h-index	580821 25 g-index
27 all docs	27 docs citations	27 times ranked	1603 citing authors

#	Article	IF	Citations
1	Correction to â€œNoncovalent Interactions by the Quantum Monte Carlo Method: Strong Influence of Isotropic Jastrow Cutoff Radiiâ€. Journal of Chemical Theory and Computation, 2022, 18, 4595-4595.	5.3	0
2	Fragmentation of natural orbital occupation numbersâ€based diagnostic of differential multireference character in complexes with hydrogen bonds. Journal of Computational Chemistry, 2021, 42, 475-483.	3.3	1
3	Noncovalent Interactions by the Quantum Monte Carlo Method: Strong Influence of Isotropic Jastrow Cutoff Radii. Journal of Chemical Theory and Computation, 2021, 17, 4242-4249.	5.3	4
4	Fundamental gap of fluorographene by many-body GW and fixed-node diffusion Monte Carlo methods. Journal of Chemical Physics, 2020, 153, 184706.	3.0	17
5	Benchmarking lattice energy of a model 1D molecular HF crystal. Theoretical Chemistry Accounts, 2020, 139, 1.	1.4	3
6	Fractional Charge by Fixed-Node Diffusion MonteÂCarlo Method. Physical Review Letters, 2019, 123, 156402.	7.8	6
7	Toward Accurate Hydrogen Bonds by Scalable Quantum Monte Carlo. Journal of Chemical Theory and Computation, 2019, 15, 3552-3557.	5.3	12
8	Room temperature organic magnets derived from sp3 functionalized graphene. Nature Communications, 2017, 8, 14525.	12.8	112
9	Bias cancellation in one-determinant fixed-node diffusion Monte Carlo: Insights from fermionic occupation numbers. Physical Review E, 2017, 95, 033308.	2.1	10
10	Noncovalent Interactions by Fixed-Node Diffusion Monte Carlo: Convergence of Nodes and Energy Differences vs Gaussian Basis-Set Size. Journal of Chemical Theory and Computation, 2017, 13, 3626-3635.	5.3	15
11	Noncovalent Interactions by QMC: Speedup by One-Particle Basis-Set Size Reduction. ACS Symposium Series, 2016, , 119-126.	0.5	1
12	Noncovalent Interactions by Quantum Monte Carlo. Chemical Reviews, 2016, 116, 5188-5215.	47.7	114
13	A Nexus between Theory and Experiment: Nonâ€Empirical Quantum Mechanical Computational Methodology Applied to Cucurbit[n]urilâ‹…Guest Binding Interactions. Chemistry - A European Journal, 2016, 22, 17226-17238.	3.3	29
14	Photocurrent spectra of semi-insulating GaAs Mâ€“Sâ€“M diodes: Role of the contacts. Solid-State Electronics, 2016, 118, 30-35.	1.4	5
15	Graphitic Nitrogen Doping in Carbon Dots Causes Red-Shifted Absorption. Journal of Physical Chemistry C, 2016, 120, 1303-1308.	3.1	207
16	Choosing a density functional for modeling adsorptive hydrogen storage: reference quantum mechanical calculations and a comparison of dispersion-corrected density functionals. Physical Chemistry Chemical Physics, 2015, 17, 6423-6432.	2.8	33
17	Extensions and applications of the A24 data set of accurate interaction energies. Physical Chemistry Chemical Physics, 2015, 17, 19268-19277.	2.8	50
18	Reactivity of Fluorographene: A Facile Way toward Graphene Derivatives. Journal of Physical Chemistry Letters, 2015, 6, 1430-1434.	4.6	90

#	Article	IF	Citations
19	Nature of Absorption Bands in Oxygen-Functionalized Graphitic Carbon Dots. Journal of Physical Chemistry C, 2015, 119, 13369-13373.	3.1	96
20	Chemical feasibility of the general acid/base mechanism of glmS ribozyme selfâ€cleavage. Biopolymers, 2015, 103, 550-562.	2.4	9
21	The work functions of Au/Mg decorated Au(100), Mg(001), and AuMg alloy surfaces: A theoretical study. Journal of Chemical Physics, 2014, 141, 094705.	3.0	6
22	Quantum Monte Carlo for noncovalent interactions: an efficient protocol attaining benchmark accuracy. Physical Chemistry Chemical Physics, 2014, 16, 20915-20923.	2.8	46
23	Quantum Monte Carlo Methods Describe Noncovalent Interactions with Subchemical Accuracy. Journal of Chemical Theory and Computation, 2013, 9, 4287-4292.	5.3	88
24	Spin-Crossing in an Organometallic Ptâ€“Benzene Complex. Journal of Chemical Theory and Computation, 2013, 9, 1461-1468.	5.3	19
25	Random Phase Approximation in Surface Chemistry: Water Splitting on Iron. Journal of Chemical Theory and Computation, 2013, 9, 3670-3676.	5.3	39
26	Magnetism in Thiolated Gold Model Junctions. Journal of Physical Chemistry C, 2012, 116, 17714-17720.	3.1	5