Claudia Filippi

List of Publications by Year
in descending order

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Version: 2024-02-01

34 papers	2,577 citations	236612 25 h-index	377514 34 g-index
36 all docs	36 docs citations	36 times ranked	1735 citing authors

#	Article	IF	Citations
1	Reference Excitation Energies of Increasingly Large Molecules: A QMC Study of Cyanine Dyes. Journal of Chemical Theory and Computation, 2022, 18, 1089-1095.	2.3	7
2	Energy Derivatives in Real-Space Diffusion Monte Carlo. Journal of Chemical Theory and Computation, 2022, 18, 118-123.	2.3	9
3	Tailoring CIPSI Expansions for QMC Calculations of Electronic Excitations: The Case Study of Thiophene. Journal of Chemical Theory and Computation, 2021, 17, 3426-3434.	2.3	17
4	Variational Principles in Quantum Monte Carlo: The Troubled Story of Variance Minimization. Journal of Chemical Theory and Computation, 2020, 16, 4203-4212.	2.3	17
5	The key to the yellow-to-cyan tuning in the green fluorescent protein family is polarisation. Physical Chemistry Chemical Physics, 2019, 21, 18988-18998.	1.3	21
6	Excited States with Selected Configuration Interaction-Quantum Monte Carlo: Chemically Accurate Excitation Energies and Geometries. Journal of Chemical Theory and Computation, 2019, 15, 4896-4906.	2.3	34
7	Taming the Complexity of Donorâ€“Acceptor Stenhouse Adducts: Infrared Motion Pictures of the Complete Switching Pathway. Journal of the American Chemical Society, 2019, 141, 7376-7384.	6.6	66
8	Photoprogramming Allostery in Human Serum Albumin. Bioconjugate Chemistry, 2018, 29, 2215-2224.	1.8	3
9	Perturbatively Selected Configuration-Interaction Wave Functions for Efficient Geometry Optimization in Quantum Monte Carlo. Journal of Chemical Theory and Computation, 2018, 14, 4176-4182.	2.3	42
10	Optimizing the Energy with Quantum Monte Carlo: A Lower Numerical Scaling for Jastrowâ€“Slater Expansions. Journal of Chemical Theory and Computation, 2017, 13, 5273-5281.	2.3	39
11	Simple formalism for efficient derivatives and multi-determinant expansions in quantum Monte Carlo. Journal of Chemical Physics, 2016, 144, 194105.	1.2	45
12	Electrostatic versus Resonance Interactions in Photoreceptor Proteins: The Case of Rhodopsin. Journal of Physical Chemistry Letters, 2016, 7, 4547-4553.	2.1	25
13	Introducing QMC/MMpol: Quantum Monte Carlo in Polarizable Force Fields for Excited States. Journal of Chemical Theory and Computation, 2016, 12, 1674-1683.	2.3	28
14	Multiple-Resonance Local Wave Functions for Accurate Excited States in Quantum Monte Carlo. Journal of Chemical Theory and Computation, 2016, 12, 1157-1168.	2.3	11
15	Chromophoreâ€“Protein Coupling beyond Nonpolarizable Models: Understanding Absorption in Green Fluorescent Protein. Journal of Chemical Theory and Computation, 2015, 11, 4825-4839.	2.3	65
16	Wavefunction in Density Functional Theory Embedding for Excited States: Which Wavefunctions, which Densities?. ChemPhysChem, 2014, 15, 3205-3217.	1.0	60
17	Solvent Effects on Excited-State Structures: A Quantum Monte Carlo and Density Functional Study. Journal of Chemical Theory and Computation, 2014, 10, 5528-5537.	2.3	12
18	Rhodopsin Absorption from First Principles: Bypassing Common Pitfalls. Journal of Chemical Theory and Computation, 2013, 9, 2441-2454.	2.3	81

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19	Ground- and Excited-State Geometry Optimization of Small Organic Molecules with Quantum Monte Carlo. Journal of Chemical Theory and Computation, 2013, 9, 5513-5525.	2.3	52
20	State-Specific Embedding Potentials for Excitation-Energy Calculations. Journal of Chemical Theory and Computation, 2013, 9, 2355-2367.	2.3	70
21	Excitation energies of retinal chromophores: critical role of the structural model. Physical Chemistry Chemical Physics, 2012, 14, 11015.	1.3	48
22	Bathochromic Shift in Green Fluorescent Protein: A Puzzle for QM/MM Approaches. Journal of Chemical Theory and Computation, 2012, 8, 112-124.	2.3	94
23	Electronic Excitations of Simple Cyanine Dyes: Reconciling Density Functional and Wave Function Methods. Journal of Chemical Theory and Computation, 2011, 7, 444-455.	2.3	124
24	Photoisomerization of Model Retinal Chromophores: Insight from Quantum Monte Carlo and Multiconfigurational Perturbation Theory. Journal of Chemical Theory and Computation, 2010, 6, 1275-1292.	2.3	126
25	Size-consistent variational approaches to nonlocal pseudopotentials: Standard and lattice regularized diffusion Monte Carlo methods revisited. Journal of Chemical Physics, 2010, 132, 154113.	1.2	102
26	Absorption Spectrum of the Green Fluorescent Protein Chromophore: A Difficult Case for ab Initio Methods?. Journal of Chemical Theory and Computation, 2009, 5, 2074-2087.	2.3	134
27	Mixed time-dependent density-functional theory/classical trajectory surface hopping study of oxirane photochemistry. Journal of Chemical Physics, 2008, 129, 124108.	1.2	182
28	Alleviation of the Fermion-Sign Problem by Optimization of Many-Body Wave Functions. Physical Review Letters, 2007, 98, 110201.	2.9	411
29	Energy and Variance Optimization of Many-Body Wave Functions. Physical Review Letters, 2005, 94, 150201.	2.9	155
30	Excitations in photoactive molecules from quantum Monte Carlo. Journal of Chemical Physics, 2004, 121, 5836-5844.	1.2	60
31	Optimized Jastrowâ€“Slater wave functions for ground and excited states: Application to the lowest states of ethene. Journal of Chemical Physics, 2004, 120, 10931-10941.	1.2	82
32	Correlated sampling in quantum Monte Carlo: A route to forces. Physical Review B, 2000, 61, R16291-R16294.	1.1	89
33	Spin contamination in quantum Monte Carlo wave functions. Journal of Chemical Physics, 1998, 108, 8838-8847.	1.2	44
34	Multiconfiguration wave functions for quantum Monte Carlo calculations of firstâ€row diatomic molecules. Journal of Chemical Physics, 1996, 105, 213-226.	1.2	213