Claudia Filippi

List of Publications by Year
in descending order

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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	Alleviation of the Fermion-Sign Problem by Optimization of Many-Body Wave Functions. Physical Review Letters, 2007, 98, 110201.	2.9	411
2	Multiconfiguration wave functions for quantum Monte Carlo calculations of firstâ€row diatomic molecules. Journal of Chemical Physics, 1996, 105, 213-226.	1.2	213
3	Mixed time-dependent density-functional theory/classical trajectory surface hopping study of oxirane photochemistry. Journal of Chemical Physics, 2008, 129, 124108.	1.2	182
4	Energy and Variance Optimization of Many-Body Wave Functions. Physical Review Letters, 2005, 94, 150201.	2.9	155
5	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
6	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
7	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
8	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
9	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
10	Correlated sampling in quantum Monte Carlo: A route to forces. Physical Review B, 2000, 61, R16291-R16294.	1.1	89
11	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
12	Rhodopsin Absorption from First Principles: Bypassing Common Pitfalls. Journal of Chemical Theory and Computation, 2013, 9, 2441-2454.	2.3	81
13	State-Specific Embedding Potentials for Excitation-Energy Calculations. Journal of Chemical Theory and Computation, 2013, 9, 2355-2367.	2.3	70
14	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
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	Excitations in photoactive molecules from quantum Monte Carlo. Journal of Chemical Physics, 2004, 121, 5836-5844.	1.2	60
17	Wavefunction in Density Functional Theory Embedding for Excited States: Which Wavefunctions, which Densities?. ChemPhysChem, 2014, 15, 3205-3217.	1.0	60
18	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

#	Article	IF	Citations
19	Excitation energies of retinal chromophores: critical role of the structural model. Physical Chemistry Chemical Physics, 2012, 14, 11015.	1.3	48
20	Simple formalism for efficient derivatives and multi-determinant expansions in quantum Monte Carlo. Journal of Chemical Physics, 2016, 144, 194105.	1.2	45
21	Spin contamination in quantum Monte Carlo wave functions. Journal of Chemical Physics, 1998, 108, 8838-8847.	1.2	44
22	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
23	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
24	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
25	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
26	Electrostatic versus Resonance Interactions in Photoreceptor Proteins: The Case of Rhodopsin. Journal of Physical Chemistry Letters, 2016, 7, 4547-4553.	2.1	25
27	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
28	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
29	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
30	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
31	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
32	Energy Derivatives in Real-Space Diffusion Monte Carlo. Journal of Chemical Theory and Computation, 2022, 18, 118-123.	2.3	9
33	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
34	Photoprogramming Allostery in Human Serum Albumin. Bioconjugate Chemistry, 2018, 29, 2215-2224.	1.8	3