Christoph Riplinger

List of Publications by Year
in descending order

23 papers	7,109 citations	393982 19 h-index	642321 23 g-index
23 all docs	23 docs citations	23 times ranked	4490 citing authors

#	Article	IF	Citations
1	Quantum computing in pharma: A multilayer embedding approach for near future applications. Journal of Computational Chemistry, 2023, 44, 406-421.	1.5	7
2	High Level Electronic Structure Calculation of Molecular Solid-State NMR Shielding Constants. Journal of Chemical Theory and Computation, 2022, 18, 2408-2417.	2.3	4
3	Unraveling individual <scp>hostâ€“guest</scp> interactions in molecular recognition from first principles quantum mechanics: Insights into the nature of nicotinic acetylcholine receptor agonist binding. Journal of Computational Chemistry, 2021, 42, 293-302.	1.5	12
4	Addressing the System-Size Dependence of the Local Approximation Error in Coupled-Cluster Calculations. Journal of Physical Chemistry A, 2021, 125, 9932-9939.	1.1	17
5	The ORCA quantum chemistry program package. Journal of Chemical Physics, 2020, 152, 224108.	1.2	1,915
6	Linear scaling perturbative triples correction approximations for open-shell domain-based local pair natural orbital coupled cluster singles and doubles theory [DLPNO-CCSD(T/T)]. Journal of Chemical Physics, 2020, 152, 024116.	1.2	50
7	Multilayer Approach to the IP-EOM-DLPNO-CCSD Method: Theory, Implementation, and Application. Journal of Chemical Theory and Computation, 2019, 15, 2265-2277.	2.3	21
8	Communication: An improved linear scaling perturbative triples correction for the domain based local pair-natural orbital based singles and doubles coupled cluster method [DLPNO-CCSD(T)]. Journal of Chemical Physics, 2018, 148, 011101.	1.2	402
9	NAMD goes quantum: an integrative suite for hybrid simulations. Nature Methods, 2018, 15, 351-354.	9.0	149
10	A near-linear scaling equation of motion coupled cluster method for ionized states. Journal of Chemical Physics, 2018, 148, 244101.	1.2	51
11	Pair natural orbital and canonical coupled cluster reaction enthalpies involving light to heavy alkali and alkaline earth metals: the importance of sub-valence correlation. Physical Chemistry Chemical Physics, 2017, 19, 9374-9391.	1.3	43
12	SparseMapsâ€”A systematic infrastructure for reduced scaling electronic structure methods. V. Linear scaling explicitly correlated coupled-cluster method with pair natural orbitals. Journal of Chemical Physics, 2017, 146, 174108.	1.2	122
13	A new near-linear scaling, efficient and accurate, open-shell domain-based local pair natural orbital coupled cluster singles and doubles theory. Journal of Chemical Physics, 2017, 146, 164105.	1.2	285
14	Multilevel Approaches within the Local Pair Natural Orbital Framework. Journal of Chemical Theory and Computation, 2017, 13, 3198-3207.	2.3	38
15	Treating Subvalence Correlation Effects in Domain Based Pair Natural Orbital Coupled Cluster Calculations: An Out-of-the-Box Approach. Journal of Chemical Theory and Computation, 2017, 13, 3220-3227.	2.3	45
16	SparseMapsâ€”A systematic infrastructure for reduced-scaling electronic structure methods. IV. Linear-scaling second-order explicitly correlated energy with pair natural orbitals. Journal of Chemical Physics, 2016, 144, 144109.	1.2	98
17	Sparse mapsâ€”A systematic infrastructure for reduced-scaling electronic structure methods. II. Linear scaling domain based pair natural orbital coupled cluster theory. Journal of Chemical Physics, 2016, 144, 024109.	1.2	740
18	Decomposition of Intermolecular Interaction Energies within the Local Pair Natural Orbital Coupled Cluster Framework. Journal of Chemical Theory and Computation, 2016, 12, 4778-4792.	2.3	231

#	Article	IF	Citations
19	Sparse mapsâ€"A systematic infrastructure for reduced-scaling electronic structure methods. I. An efficient and simple linear scaling local MP2 method that uses an intermediate basis of pair natural orbitals. Journal of Chemical Physics, 2015, 143, 034108.	1.2	211
20	Natural triple excitations in local coupled cluster calculations with pair natural orbitals. Journal of Chemical Physics, 2013, 139, 134101.	1.2	1,240
21	An efficient and near linear scaling pair natural orbital based local coupled cluster method. Journal of Chemical Physics, 2013, 138, 034106.	1.2	1,276
22	The Reaction Mechanism of Cytochrome P450 NO Reductase: A Detailed Quantum Mechanics/Molecular Mechanics Study. ChemPhysChem, 2011, 12, 3192-3203.	1.0	36
23	Interaction of Radical Pairs Through-Bond and Through-Space: Scope and Limitations of the Pointâ^'Dipole Approximation in Electron Paramagnetic Resonance Spectroscopy. Journal of the American Chemical Society, 2009, 131, 10092-10106.	6.6	116