Manuel Sparta

List of Publications by Year
in descending order

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30 papers	1,725 citations	394421 19 h-index	454955 30 g-index
32 all docs	32 docs citations	32 times ranked	1882 citing authors

#	Article	IF	Citations
1	Exploring the Accuracy Limits of Local Pair Natural Orbital Coupled-Cluster Theory. Journal of Chemical Theory and Computation, 2015, 11, 1525-1539.	5.3	544
2	Decomposition of Intermolecular Interaction Energies within the Local Pair Natural Orbital Coupled Cluster Framework. Journal of Chemical Theory and Computation, 2016, 12, 4778-4792.	5.3	231
3	Chemical applications carried out by local pair natural orbital based coupled-cluster methods. Chemical Society Reviews, 2014, 43, 5032-5041.	38.1	117
4	Activity of Rhodium-Catalyzed Hydroformylation:Â Added Insight and Predictions from Theory. Journal of the American Chemical Society, 2007, 129, 8487-8499.	13.7	94
5	An adaptive density-guided approach for the generation of potential energy surfaces of polyatomic molecules. Theoretical Chemistry Accounts, 2009, 123, 413-429.	1.4	73
6	B₁₃⁺: A Photodriven Molecular Wankel Engine. Angewandte Chemie - International Edition, 2012, 51, 8512-8515.	13.8	72
7	New Formulation and Implementation of Vibrational Self-Consistent Field Theory. Journal of Chemical Theory and Computation, 2010, 6, 235-248.	5.3	69
8	Mechanism of Olefin Asymmetric Hydrogenation Catalyzed by Iridium Phosphino-Oxazoline: A Pair Natural Orbital Coupled Cluster Study. Journal of Chemical Theory and Computation, 2014, 10, 1099-1108.	5.3	63
9	Vibrational coupled cluster response theory: A general implementation. Journal of Chemical Physics, 2011, 134, 054119.	3.0	52
10	Using Electronic Energy Derivative Information in Automated Potential Energy Surface Construction for Vibrational Calculations. Journal of Chemical Theory and Computation, 2010, 6, 3162-3175.	5.3	39
11	Multilevel Approaches within the Local Pair Natural Orbital Framework. Journal of Chemical Theory and Computation, 2017, 13, 3198-3207.	5.3	38
12	Toward Accurate QM/MM Reaction Barriers with Large QM Regions Using Domain Based Pair Natural Orbital Coupled Cluster Theory. Journal of Chemical Theory and Computation, 2018, 14, 3524-3531.	5.3	37
13	The use of local orbitals in multireference calculations. Molecular Physics, 2003, 101, 1389-1398.	1.7	36
14	Potential Energy Surfaces for Vibrational Structure Calculations from a Multiresolution Adaptive Density-Guided Approach: Implementation and Test Calculations. Journal of Physical Chemistry A, 2009, 113, 8712-8723.	2.5	34
15	Metal-Dependent Activity of Fe and Ni Acireductone Dioxygenases: How Two Electrons Reroute the Catalytic Pathway. Journal of Molecular Biology, 2013, 425, 3007-3018.	4.2	34
16	Accurate multimode vibrational calculations using a B-spline basis: theory, tests and application to dioxirane and diazirinone. Molecular Physics, 2011, 109, 673-685.	1.7	33
17	Hybrid Dynamics Simulation Engine for Metalloproteins. Biophysical Journal, 2012, 103, 767-776.	0.5	26
18	How Metal Substitution Affects the Enzymatic Activity of Catechol-O-Methyltransferase. PLoS ONE, 2012, 7, e47172.	2.5	23

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19	The Role of the Flexible L43-S54 Protein Loop in the CcrA Metallo-Î²-lactamase in Binding Structurally Dissimilar Î²-Lactam Antibiotics. Journal of Chemical Theory and Computation, 2013, 9, 730-737.	5.3	21
20	Developments in then-electron valence state perturbation theory. International Journal of Quantum Chemistry, 2006, 106, 686-691.	2.0	13
21	Structure and Stability of Substitutional Metallofullerenes of the Firstâ€Row Transition Metals. Fullerenes Nanotubes and Carbon Nanostructures, 2006, 14, 269-278.	2.1	12
22	Structure and Stability of Networked Metallofullerenes of the Transition Metals. Journal of Physical Chemistry A, 2006, 110, 11711-11716.	2.5	11
23	Vibrational spectroscopy of hydrogen-bonded systems: Six-dimensional simulation of the IR spectrum of Fâ¯(H2O) complex. Chemical Physics Letters, 2011, 510, 36-41.	2.6	10
24	Accurate metalâ€“ligand bond energies in the Î·²-C₂H₄ and Î·²-C₆₀ complexes of Pt(PH₃)₂, with application to their Bis(triphenylphosphine) analogues. Molecular Physics, 2013, 111, 1599-1611.	1.7	8
25	Skin and Proximity Effects in Electrodes and Furnace Shells. Metallurgical and Materials Transactions B: Process Metallurgy and Materials Processing Science, 2019, 50, 2884-2897.	2.1	8
26	IR, Raman and SERS spectra of propantheline bromide. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 103, 1-10.	3.9	6
27	Computational design and characterisation of artificial enzymes for Kemp elimination. Molecular Simulation, 2011, 37, 557-571.	2.0	5
28	Metamodeling of the Electrical Conditions in Submerged Arc Furnaces. Metallurgical and Materials Transactions B: Process Metallurgy and Materials Processing Science, 2021, 52, 1267-1278.	2.1	5
29	A priori complete active space self consistent field localized orbitals: an application on linear polyenes. Molecular Physics, 2006, 104, 691-700.	1.7	3
30	An Overall Furnace Model for the Silicomanganese Process. Jom, 2021, 73, 2672-2681.	1.9	0