Dimitrios G Liakos

List of Publications by Year
in descending order

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Version: 2024-02-01

28 papers	2,812 citations	448610 19 h-index	591227 27 g-index
30 all docs	30 docs citations	30 times ranked	2575 citing authors

#	Article	IF	Citations
1	Short-Range Disorder in TeO₂ Melt and Glass. Journal of Physical Chemistry Letters, 2020, 11, 427-431.	2.1	22
2	Comprehensive Benchmark Results for the Domain Based Local Pair Natural Orbital Coupled Cluster Method (DLPNO-CCSD(T)) for Closed- and Open-Shell Systems. Journal of Physical Chemistry A, 2020, 124, 90-100.	1.1	169
3	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
4	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
5	Exploring the Accuracy Limits of Local Pair Natural Orbital Coupled-Cluster Theory. Journal of Chemical Theory and Computation, 2015, 11, 1525-1539.	2.3	544
6	Is It Possible To Obtain Coupled Cluster Quality Energies at near Density Functional Theory Cost? Domain-Based Local Pair Natural Orbital Coupled Cluster vs Modern Density Functional Theory. Journal of Chemical Theory and Computation, 2015, 11, 4054-4063.	2.3	248
7	Domain Based Pair Natural Orbital Coupled Cluster Studies on Linear and Folded Alkane Chains. Journal of Chemical Theory and Computation, 2015, 11, 2137-2143.	2.3	57
8	On the Reaction Mechanism of the Complete Intermolecular O₂ Transfer between Mononuclear Nickel and Manganese Complexes with Macrocyclic Ligands. Chemistry - A European Journal, 2014, 20, 13296-13304.	1.7	7
9	Excitation Wavelength Dependent O₂ Release from Copper(II)â€“Superoxide Compounds: Laser Flash-Photolysis Experiments and Theoretical Studies. Journal of the American Chemical Society, 2014, 136, 1260-1263.	6.6	34
10	Kubas complexes extended to four centers; a theoretical prediction ofÂnovel dihydrogen coordination in bimetallic tungsten and molybdenum compounds. Journal of Organometallic Chemistry, 2014, 766, 67-72.	0.8	2
11	Theoretical prediction of new Kubas four centre H2 complexes involving dimolybdate clusters. Chemical Physics Letters, 2013, 583, 18-22.	1.2	5
12	What is the most efficient way to reach the canonical MP2 basis set limit?. Molecular Physics, 2013, 111, 2653-2662.	0.8	33
13	Theoretical Elucidation of a Classic Reaction: Protonation of the Quadruple Bond of the Octachlorodimolybdate(II,II) [Mo₂Cl₈]^{4â€“} Anion. Inorganic Chemistry, 2012, 51, 258-266.	1.9	5
14	Improved Correlation Energy Extrapolation Schemes Based on Local Pair Natural Orbital Methods. Journal of Physical Chemistry A, 2012, 116, 4801-4816.	1.1	95
15	Weak Molecular Interactions Studied with Parallel Implementations of the Local Pair Natural Orbital Coupled Pair and Coupled Cluster Methods. Journal of Chemical Theory and Computation, 2011, 7, 76-87.	2.3	140
16	Proteinâ€“Ligand Interaction Energies with Dispersion Corrected Density Functional Theory and High-Level Wave Function Based Methods. Journal of Physical Chemistry A, 2011, 115, 11210-11220.	1.1	78
17	Efficient and accurate local single reference correlation methods for high-spin open-shell molecules using pair natural orbitals. Journal of Chemical Physics, 2011, 135, 214102.	1.2	165
18	Interplay of Correlation and Relativistic Effects in Correlated Calculations on Transition-Metal Complexes: The (Cu₂O₂)²⁺ Core Revisited. Journal of Chemical Theory and Computation, 2011, 7, 1511-1523.	2.3	104

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19	Correlated wavefunction methods in bioinorganic chemistry. Journal of Biological Inorganic Chemistry, 2011, 16, 821-829.	1.1	47
20	Dealing with Complexity in Open-Shell Transition Metal Chemistry from a Theoretical Perspective: Reaction Pathways, Bonding, Spectroscopy, And Magnetic Properties. Advances in Inorganic Chemistry, 2010, 62, 301-349.	0.4	36
21	A Multiconfigurational ab Initio Study of the Zero-Field Splitting in the Di- and Trivalent Hexaquoâ^'Chromium Complexes. Inorganic Chemistry, 2009, 48, 10572-10580.	1.9	54
22	Efficient and accurate approximations to the local coupled cluster singles doubles method using a truncated pair natural orbital basis. Journal of Chemical Physics, 2009, 131, 064103.	1.2	468
23	Structural properties of lithium metaphosphate glasses by ab initio molecular electronic structure calculations. Journal of Non-Crystalline Solids, 2008, 354, 1569-1574.	1.5	3
24	Theoretical Study of Glass Systems using Molecular Electronic Structure Theory. 2. Structure and Spectroscopy of the B₂O₃ Glass. Journal of Physical Chemistry A, 2008, 112, 7881-7886.	1.1	9
25	Theoretical Investigation of the Stepwise Hydrolysis of the [Re3(Î¼-Cl)3Cl9]3-Anion. Inorganic Chemistry, 2007, 46, 2167-2172.	1.9	1
26	Theoretical Study of Glass Systems Using ab initio Molecular Electronic Structure Theory. Part 1. Lithium Metaphosphate Glass.. ChemInform, 2004, 35, no.	0.1	0
27	Theoretical Study of Glass Systems Using ab Initio Molecular Electronic Structure Theory. 1. Lithium Metaphosphate Glass. Journal of Physical Chemistry A, 2004, 108, 3854-3858.	1.1	8
28	A theoretical study on the solvolytic reactivity of the [Re3(Î¼-Cl3)Cl9]nâ^' clusters (n=3,4) using ab initio and density functional theory calculations. Chemical Physics Letters, 2003, 369, 490-494.	1.2	26