Konstantinos D Vogiatzis

List of Publications by Year
in descending order

60 papers	3,099 citations	201385 27 h-index	155451 55 g-index
65 all docs	65 docs citations	65 times ranked	4491 citing authors

#	Article	IF	Citations
1	NWChem: Past, present, and future. Journal of Chemical Physics, 2020, 152, 184102.	1.2	425
2	Advances, Updates, and Analytics for the Computation-Ready, Experimental Metalâ€“Organic Framework Database: CoRE MOF 2019. Journal of Chemical & Engineering Data, 2019, 64, 5985-5998.	1.0	372
3	Computational Approach to Molecular Catalysis by 3d Transition Metals: Challenges and Opportunities. Chemical Reviews, 2019, 119, 2453-2523.	23.0	260
4	Ab initio Study of the Interactions between CO₂ and Nâ€Containing Organic Heterocycles. ChemPhysChem, 2009, 10, 374-383.	1.0	180
5	Catalytic Silylation of Dinitrogen with a Dicobalt Complex. Journal of the American Chemical Society, 2015, 137, 4638-4641.	6.6	162
6	Superstretchable, Selfâ€Healing Polymeric Elastomers with Tunable Properties. Advanced Functional Materials, 2018, 28, 1800741.	7.8	162
7	Mechanism of Oxidation of Ethane to Ethanol at Iron(IV)â€“Oxo Sites in Magnesium-Diluted Fe₂(dobdc). Journal of the American Chemical Society, 2015, 137, 5770-5781.	6.6	156
8	Pushing configuration-interaction to the limit: Towards massively parallel MCSCF calculations. Journal of Chemical Physics, 2017, 147, 184111.	1.2	120
9	Selective, Tunable O₂ Binding in Cobalt(II)â€“Triazolate/Pyrazolate Metalâ€“Organic Frameworks. Journal of the American Chemical Society, 2016, 138, 7161-7170.	6.6	101
10	Ab Initio Derived Force Fields for Predicting CO₂ Adsorption and Accessibility of Metal Sites in the Metalâ€“Organic Frameworks M-MOF-74 (M = Mn, Co, Ni, Cu). Journal of Physical Chemistry C, 2015, 119, 16058-16071.	1.5	84
11	Electronic Structure of the [Cu₃(Î¼-O)₃]²⁺ Cluster in Mordenite Zeolite and Its Effects on the Methane to Methanol Oxidation. Journal of Physical Chemistry C, 2017, 121, 22295-22302.	1.5	74
12	Representation of molecular structures with persistent homology for machine learning applications in chemistry. Nature Communications, 2020, 11, 3230.	5.8	61
13	Ab Initio Study of the Adsorption of Small Molecules on Metalâ€“Organic Frameworks with Oxo-centered Trimetallic Building Units: The Role of the Undercoordinated Metal Ion. Inorganic Chemistry, 2015, 54, 8251-8263.	1.9	48
14	Systematic Expansion of Active Spaces beyond the CASSCF Limit: A GASSCF/SplitGAS Benchmark Study. Journal of Chemical Theory and Computation, 2015, 11, 3010-3021.	2.3	48
15	Accelerated Computational Analysis of Metalâ€“Organic Frameworks for Oxidation Catalysis. Journal of Physical Chemistry C, 2016, 120, 18707-18712.	1.5	44
16	Unprecedented Fiveâ€Coordinate Iron(IV) Imides Generate Divergent Spin States Based on the Imide Râ€Groups. Angewandte Chemie - International Edition, 2019, 58, 8115-8118.	7.2	44
17	Elimination of CO₂/N₂ Langmuir Sorption and Promotion of â€œN₂-Phobicityâ€•within High-T_g Glassy Membranes. Macromolecules, 2019, 52, 1589-1600.	2.2	43
18	Elastic Single-Ion Conducting Polymer Electrolytes: Toward a Versatile Approach for Intrinsically Stretchable Functional Polymers. Macromolecules, 2020, 53, 3591-3601.	2.2	41

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19	Data-Driven Acceleration of the Coupled-Cluster Singles and Doubles Iterative Solver. Journal of Physical Chemistry Letters, 2019, 10, 4129-4135.	2.1	39
20	Thermodynamic and kinetic studies of H₂ and N₂ binding to bimetallic nickel-group 13 complexes and neutron structure of a Ni(Î·²-H₂) adduct. Chemical Science, 2019, 10, 7029-7042.	3.7	38
21	Adhesive Polymers as Efficient Binders for High-Capacity Silicon Electrodes. ACS Applied Energy Materials, 2020, 3, 3387-3396.	2.5	34
22	Computational catalysis for metal-organic frameworks: An overview. Coordination Chemistry Reviews, 2021, 436, 213777.	9.5	34
23	Non-covalent Interactions of CO₂ with Functional Groups of Metalâ€“Organic Frameworks from a CCSD(T) Scheme Applicable to Large Systems. Journal of Chemical Theory and Computation, 2015, 11, 1574-1584.	2.3	32
24	Accurate atomization energies from combining coupled-cluster computations with interference-corrected explicitly correlated second-order perturbation theory. Theoretical Chemistry Accounts, 2014, 133, 1.	0.5	29
25	Ligand field effects on the ground and excited states of reactive FeO²⁺ species. Physical Chemistry Chemical Physics, 2018, 20, 28786-28795.	1.3	29
26	Selective Catalytic Chemistry at Rhodium(II) Nodes in Bimetallic Metalâ€“Organic Frameworks. Angewandte Chemie - International Edition, 2019, 58, 16533-16537.	7.2	29
27	Magnetic Properties of Paddlewheels and Trinuclear Clusters with Exposed Metal Sites. ChemPhysChem, 2011, 12, 3307-3319.	1.0	27
28	Addition-type alkoxysilyl-substituted polynorbornenes for post-combustion carbon dioxide separations. Journal of Membrane Science, 2020, 595, 117532.	4.1	27
29	Bi- and trimetallic rare-earthâ€“palladium complexes ligated by phosphinoamides. Chemical Communications, 2015, 51, 11761-11764.	2.2	26
30	Interference-corrected explicitly-correlated second-order perturbation theory. Chemical Physics Letters, 2011, 503, 157-161.	1.2	25
31	Quantum Chemical Characterization of Single Molecule Magnets Based on Uranium. Journal of Physical Chemistry A, 2017, 121, 1726-1733.	1.1	25
32	Gas separation mechanism of CO₂ selective amidoxime-poly(1-trimethylsilyl-1-propyne) membranes. Polymer Chemistry, 2017, 8, 3341-3350.	1.9	25
33	Accurate computations of the structures and binding energies of the imidazole<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si45.gif" overflow="scroll"><mml:mrow><mml:mo>â‹¯</mml:mo></mml:mrow></mml:math>benzene and pyrrole<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si46.gif" overflow="scroll"><mml:mrow><mml:mo>â‹¯</mml:mo></mml:mrow></mml:math>benzene complexes. Chemical Physics, 2014, 441, 17-22.	0.9	22
34	Catechol-Ligated Transition Metals: A Quantum Chemical Study on a Promising System for Gas Separation. Journal of Physical Chemistry C, 2017, 121, 10463-10469.	1.5	20
35	Electrocatalytic Dechlorination of Dichloromethane in Water Using a Heterogenized Molecular Copper Complex. Inorganic Chemistry, 2021, 60, 4915-4923.	1.9	20
36	Post-Hartree-Fock methods: configuration interaction, many-body perturbation theory, coupled-cluster theory. , 2019, , 63-117.		17

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37	Direct Identification of Mixed-Metal Centers in Metalâ€“Organic Frameworks: Cu₃(BTC)₂ Transmetalated with Rh²⁺ Ions. Journal of Physical Chemistry Letters, 2020, 11, 8138-8144.	2.1	16
38	Accurate non-covalent interactions with basis-set corrections from interference-corrected perturbation theory: comparison with the S22B database. Molecular Physics, 2013, 111, 2299-2305.	0.8	15
39	Transferable MP2-Based Machine Learning for Accurate Coupled-Cluster Energies. Journal of Chemical Theory and Computation, 2020, 16, 7453-7461.	2.3	14
40	Unprecedented Fiveâ€Coordinate Iron(IV) Imides Generate Divergent Spin States Based on the Imide Râ€Groups. Angewandte Chemie, 2019, 131, 8199-8202.	1.6	13
41	Selecting Quantum-Chemical Methods for Lanthanide-Containing Molecules: A Balance between Accuracy and Efficiency. Inorganic Chemistry, 2020, 59, 10492-10500.	1.9	13
42	CO₂ Capture on Functionalized Calixarenes: A Computational Study. Journal of Physical Chemistry A, 2019, 123, 10116-10122.	1.1	10
43	Evaluating the impact of functional groups on membraneâ€mediated <scp>CO₂</scp>/<scp>N₂</scp> gas separations using a common polymer backbone. Journal of Polymer Science, 2020, 58, 2644-2653.	2.0	10
44	Pushing Single-Oxygen-Atom-Bridged Bimetallic Systems to the Right: A Cryptand-Encapsulated Coâ€“Oâ€“Co Unit. Journal of the American Chemical Society, 2015, 137, 15354-15357.	6.6	9
45	Gas-Phase Ion Chemistry of Metalloporphyrin Anions with Molecular Oxygen: Probing the Influence of the Oxidation and Spin State of the Central Transition Metal by Experiment and Theory. Journal of Physical Chemistry A, 2018, 122, 4357-4365.	1.1	8
46	Vinyl-Addition Fluoroalkoxysilyl-Substituted Polynorbornene Membranes for CO₂/CH₄ Separation. ACS Applied Polymer Materials, 2022, 4, 7976-7988.	2.0	8
47	A PEGylated Tin Porphyrin Complex for Electrocatalytic Proton Reduction: Mechanistic Insights into Mainâ€Groupâ€Element Catalysis. Angewandte Chemie - International Edition, 2022, 61, .	7.2	8
48	Selective Catalytic Chemistry at Rhodium(II) Nodes in Bimetallic Metalâ€“Organic Frameworks. Angewandte Chemie, 2019, 131, 16685-16689.	1.6	7
49	A Carbodiimide-Mediated Pâ€“C Bond-Forming Reaction: Mild Amidoalkylation of P-Nucleophiles by Boc-Aminals. Organic Letters, 2021, 23, 1726-1730.	2.4	7
50	Electrocatalytic Hydrogen Evolution Using A Molecular Antimony Complex under Aqueous Conditions: An Experimental and Computational Study on Mainâ€Group Element Catalysis. Chemistry - A European Journal, 2022, 28, .	1.7	7
51	Understanding the Nature of Weak Interactions between Functionalized Boranes and N₂/O₂, Promising Functional Groups for Gas Separations. Journal of Physical Chemistry A, 2019, 123, 3315-3325.	1.1	6
52	Ïƒ-Donation and Ï€-Backdonation Effects in Dative Bonds of Main-Group Elements. Journal of Physical Chemistry A, 2021, 125, 7956-7966.	1.1	5
53	Ion specific fluorescence modulation of polyvinyl alcohol-boronate matrices. Polymer Chemistry, 2020, 11, 1919-1925.	1.9	4
54	Potent Anti-Inflammatory, Arylpyrazole-Based Glucocorticoid Receptor Agonists That Do Not Impair Insulin Secretion. ACS Medicinal Chemistry Letters, 2021, 12, 1568-1577.	1.3	3

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55	Mechanistic Investigations of Gas-Phase Catalytic Hydrogenation in Metalâ€“Organic Frameworks: Cooperative Activity of the Metal and Linker Sites in Cu_xRh_{3â€“x}(BTC)₂. Journal of Physical Chemistry C, 2022, 126, 11553-11565.	1.5	3
56	Redox states of dinitrogen coordinated to a molybdenum atom. Journal of Chemical Physics, 2021, 154, 224308.	1.2	2
57	Nature of the Short Rhâ€“Li Contact between Lithium and the Rhodium Ï‰-Alkenyl Complex [Rh(CH₂CMe₂CH₂CHâ•CH₂)₂]^{â^’}. Inorganic Chemistry, 2021, 60, 8790-8801.	1.9	2
58	Correction to â€œCatechol-Ligated Transition Metals: A Quantum Chemical Study on a Promising System for Gas Separationâ€. Journal of Physical Chemistry C, 2017, 121, 20553-20553.	1.5	1
59	On the Interaction between Carbon Dioxide and Nanomaterials with High Accuracy ab initio and DFT Calculations. , 2009, , .		0
60	A PEGylated Tinâ€Porphyrin Complex for Electrocatalytic Proton Reduction: Mechanistic Insights into Mainâ€Group Element Catalysis. Angewandte Chemie, 0, , .	1.6	0