Mohammad Reza Momeni Taheri

List of Publications by Year
in descending order

49 papers	1,242 citations	489802 18 h-index	425179 34 g-index
55 all docs	55 docs citations	55 times ranked	1729 citing authors

#	Article	IF	Citations
1	Modeling energy transfer and absorption spectra in layered metal-organic frameworks based on a Frenkel-Holstein Hamiltonian. Journal of Chemical Physics, 2022, 156, 044109.	1.2	1
2	Metal-to-Semiconductor Transition in Two-Dimensional Metalâ€“Organic Frameworks: An Ab Initio Dynamics Perspective. ACS Applied Materials & Interfaces, 2021, 13, 25270-25279.	4.0	8
3	Tuning electronic properties of conductive 2D layered metalâ€“organic frameworks via hostâ€“guest interactions: Dioxygen as an electroactive chemical stimuli. APL Materials, 2021, 9, .	2.2	7
4	Gauging van der Waals interactions in aqueous solutions of 2D MOFs: when water likes organic linkers more than open-metal sites. Physical Chemistry Chemical Physics, 2021, 23, 3135-3143.	1.3	6
5	Deterministic role of structural flexibility on catalytic activity of conductive 2D layered metalâ€“organic frameworks. Chemical Communications, 2021, 57, 315-318.	2.2	6
6	Water-Induced Structural Transformations in Flexible Two-Dimensional Layered Conductive Metalâ€“Organic Frameworks. Chemistry of Materials, 2020, 32, 9664-9674.	3.2	15
7	Computational Screening of Roles of Defects and Metal Substitution on Reactivity of Different Single- vs Double-Node Metalâ€“Organic Frameworks for Sarin Decomposition. Journal of Physical Chemistry C, 2019, 123, 15157-15165.	1.5	31
8	Halogen bonding in UiO-66 frameworks promotes superior chemical warfare agent simulant degradation. Chemical Communications, 2019, 55, 3481-3484.	2.2	68
9	Correction to â€œTuning Zr₆ Metal-Organic Framework (MOF) Nodes as Catalyst Supports: Site Densities and Electron-Donor Properties Influence Molecular Iridium Complexes as Ethylene Conversion Catalystsâ€. ACS Catalysis, 2018, 8, 2364-2364.	5.5	3
10	Dual Role of Water in Heterogeneous Catalytic Hydrolysis of Sarin by Zirconium-Based Metalâ€“Organic Frameworks. ACS Applied Materials & Interfaces, 2018, 10, 18435-18439.	4.0	62
11	Density Functional Modeling of Ligand Effects on Electronic Structure and Câ€“H Bond Activation Activity of Copper(III) Hydroxide Compounds. Inorganic Chemistry, 2018, 57, 9807-9813.	1.9	8
12	Structural Characterization of Pristine and Defective [Zr₁₂(Î¼₃-O)₈(Î¼₃-OH)₈(Î¼₂-OH)₆(sub Double-Node Metalâ€“Organic Framework and Predicted Applications for Single-Site Catalytic Hydrolysis of Sarin. Chemistry of Materials, 2018, 30, 4432-4439.	3.2	42
13	Tuning the properties of metalâ€“organic framework nodes as supports of single-site iridium catalysts: node modification by atomic layer deposition of aluminium. Faraday Discussions, 2017, 201, 195-206.	1.6	30
14	A Local CC2 and TDA-DFT Double Hybrid Study on BODIPY/aza-BODIPY Dimers as Heavy Atom Free Triplet Photosensitizers for Photodynamic Therapy Applications. Journal of Physical Chemistry A, 2016, 120, 2550-2560.	1.1	52
15	Intramolecular Singlet Fission in Quinoidal Bi- and Tetrathiophenes: A Comparative Study of Low-Lying Excited Electronic States and Potential Energy Surfaces. Journal of Chemical Theory and Computation, 2016, 12, 5067-5075.	2.3	17
16	Toward unsaturated stannylenes Y₂Zî€Sn: and related compounds with triplet electronic ground states. RSC Advances, 2016, 6, 53749-53759.	1.7	4
17	Interplay of donorâ€“acceptor interactions in stabilizing boron nitride compounds: insights from theory. Physical Chemistry Chemical Physics, 2015, 17, 16525-16535.	1.3	13
18	Why Do TD-DFT Excitation Energies of BODIPY/Aza-BODIPY Families Largely Deviate from Experiment? Answers from Electron Correlated and Multireference Methods. Journal of Chemical Theory and Computation, 2015, 11, 2619-2632.	2.3	166

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19	Accessing Zinc Monohydride Cations through Coordinative Interactions. Angewandte Chemie - International Edition, 2014, 53, 9347-9351.	7.2	111
20	Carbene-Bound Borane and Silane Adducts: A Comprehensive DFT Study on Their Stability and Propensity for Hydride-Mediated Ring Expansion. Organometallics, 2013, 32, 6201-6208.	1.1	82
21	Estimating the stability and reactivity of acyclic and cyclic mono-heteroatom substituted germylenes: A density functional theory investigation. Computational and Theoretical Chemistry, 2013, 1009, 81-85.	1.1	9
22	Stable Complexes of Parent Digermene: An Inorganic Analogue of Ethylene. Organometallics, 2013, 32, 6658-6665.	1.1	62
23	Controlled Growth of Dichlorogermanium Oligomers from Lewis Basic Hosts. Angewandte Chemie - International Edition, 2013, 52, 6390-6395.	7.2	77
24	THEORETICAL STUDY OF HIGHLY DOPED HETEROFULLERENES EVOLVED FROM THE D6h SYMMETRY C36 CAGE. Journal of Theoretical and Computational Chemistry, 2013, 12, 1350067.	1.8	0
25	Controlled Growth of Dichlorogermanium Oligomers from Lewis Basic Hosts. Angewandte Chemie, 2013, 125, 6518-6523.	1.6	24
26	Beyond conventional N-heterocyclic silylenes: A density functional approach toward structural features and catalytic applications. Computational and Theoretical Chemistry, 2012, 985, 62-66.	1.1	0
27	A DFT study on the structural and electronic properties of Td and C2 symmetry C24X4 and C22X6 heterofullerenes (X=B, Al, N, and P). Computational and Theoretical Chemistry, 2012, 994, 14-18.	1.1	4
28	Theoretical study of highly doped heterofullerenes evolved from the smallest fullerene cage. Structural Chemistry, 2012, 23, 1503-1508.	1.0	7
29	[n]Imperilenes: Stacked [n]Trannulenes Separated by Planar Cycloalkane Rings. Organic Letters, 2011, 13, 3600-3603.	2.4	3
30	Theoretical Description of Triplet Silylenes Evolved from H₂Siâ•Si. Organometallics, 2011, 30, 5027-5032.	1.1	13
31	New Generation of Dialkylsilylenes with Stabilities Comparable to Diaminosilylenes: A Theoretical Study. Journal of Physical Chemistry A, 2011, 115, 10550-10555.	1.1	6
32	Isolation: A strategy for obtaining highly doped heterofullerenes. Chemical Physics Letters, 2011, 514, 321-324.	1.2	10
33	Stable Î±-heteroatom-free dialkylcarbenes: a DFT study. Structural Chemistry, 2011, 22, 141-147.	1.0	2
34	From acyclic dialkylcarbene to the unsaturated cyclic heteroatom substituted ones: a survey of stability. Journal of Physical Organic Chemistry, 2011, 24, 351-359.	0.9	14
35	Effects of Î±â€cyclopropyl on heterocyclic carbenes stability at DFT. Journal of Physical Organic Chemistry, 2011, 24, 1022-1029.	0.9	7
36	Monoheteroatom substituted six-membered carbenes: A computational survey of stability and reactivity. Computational and Theoretical Chemistry, 2011, 965, 101-106.	1.1	2

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37	Density functional investigation of metal encapsulated X@C12Si8 heterofullerene (X=Li+, Na+, K+,) Tj ETQq1 1 0.784314 rgBT /Overl	1.3	7
38	Stable silylenes with acyclic, cyclic, and unsaturated cyclic structures: Effects of heteroatoms and cyclopropyl Î±-substituents at DFT. Journal of Organometallic Chemistry, 2011, 696, 2059-2064.	0.8	11
39	Stable C20â^'nSin heterofullerenes (nâ©½8): A DFT approach. Chemical Physics Letters, 2010, 492, 137-141.	1.2	25
40	Novel Î±-spirocyclic (alkyl)(amino)carbenes at the theoretical crossroad of flexibility and rigidity. Structural Chemistry, 2010, 21, 593-598.	1.0	31
41	Pyridine derived N-heterocyclic germylenes: A density functional perspective. Journal of Organometallic Chemistry, 2010, 695, 760-765.	0.8	8
42	Carbenes with Reduced Heteroatom Stabilization: A Computational Approach. Journal of Organic Chemistry, 2010, 75, 2539-2545.	1.7	47
43	Silabenzene through divalent precursors at theoretical levels. Monatshefte FÃ¼r Chemie, 2009, 140, 33-38.	0.9	8
44	Toward stable N-heterocyclic silylenes at theoretical levels. Computational and Theoretical Chemistry, 2009, 913, 16-21.	1.5	10
45	Effects of fused benzene rings on tautomerizations and inversions of benzo, azabenzo, and oxabenzocycloheptatrienes at theoretical levels. Structural Chemistry, 2009, 20, 517-524.	1.0	3
46	A theoretical investigation into dimethylcarbene and its diamino and diphosphino analogs: effects of cyclization and unsaturation on the stability and multiplicity. Journal of Physical Organic Chemistry, 2009, 22, 919-924.	0.9	28
47	A DFT study on pyridine-derived N-heterocyclic carbenes. Tetrahedron, 2009, 65, 10093-10098.	1.0	36
48	A novel triplet germylene F3CGeGeH at theoretical levels. Computational and Theoretical Chemistry, 2009, 899, 46-53.	1.5	3
49	How steric effects favor thiepins over their benzene sulfide tautomers at theoretical levels?. Computational and Theoretical Chemistry, 2008, 861, 117-121.	1.5	13