Evangelos Miliordos

List of Publications by Year
in descending order

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87 papers	1,759 citations	279798 23 h-index	330143 37 g-index
90 all docs	90 docs citations	90 times ranked	1580 citing authors

#	Article	IF	Citations
1	Molecular-level electrocatalytic CO₂ reduction reaction mediated by single platinum atoms. Physical Chemistry Chemical Physics, 2022, 24, 4226-4231.	2.8	3
2	Can boron form coordination complexes with diffuse electrons? Evidence for linked solvated electron precursors. Electronic Structure, 2022, 4, 015001.	2.8	5
3	Simultaneous CO₂ capture and functionalization: solvated electron precursors as novel catalysts. Chemical Communications, 2022, 58, 1310-1313.	4.1	5
4	Ab initio investigation of the ground and excited states of TcO+ and RhO+. Journal of Quantitative Spectroscopy and Radiative Transfer, 2022, 280, 108074.	2.3	0
5	Electronic structure of the ground and excited states of neutral and charged silicon hydrides, SiH_x^{0/+/â^’}, x = 1â€“4. Physical Chemistry Chemical Physics, 2022, , .	2.8	0
6	The nature of supermolecular bonds: Investigating hydrocarbon linked beryllium solvated electron precursors. Journal of Chemical Physics, 2022, 156, .	3.0	5
7	Highly Diastereoâ€•and Enantioselective Synthesis of 3,6â€²â€Bisborylâ€•anti â€1,2â€oxaborinanâ€3â€ene: An Entry to Enantioenriched Homoallylic Alcohols with A Stereodefined Trisubstituted Alkene. Angewandte Chemie, 2021, 133, 853-861.	2.0	6
8	Ground and excited states analysis of alkali metal ethylenediamine and crown ether complexes. Physical Chemistry Chemical Physics, 2021, 23, 20298-20306.	2.8	6
9	Electronic structure of the dicationic first row transition metal oxides. Physical Chemistry Chemical Physics, 2021, 23, 21172-21182.	2.8	5
10	Infrared spectroscopy of RGâ€“Co+(H2O) complexes (RG = Ar, Ne, He): The role of rare gas â€œtagâ€•atoms. Journal of Chemical Physics, 2021, 154, 064306.	3.0	7
11	Methane to Methanol Conversion Facilitated by Anionic Transition Metal Centers: The Case of Fe, Ni, Pd, and Pt. Journal of Physical Chemistry A, 2021, 125, 2364-2373.	2.5	11
12	Electronic and geometric structure of cationic and neutral chromium and molybdenum ammonia complexes. Journal of Chemical Physics, 2021, 155, 014303.	3.0	9
13	Comparing coordination uranyl(<scp>vi</scp>) complexes with 2-(1H-imidazo[4,5-b]phenazin-2-yl)phenol and derivatives. Dalton Transactions, 2021, 50, 11113-11122.	3.3	2
14	Radical abstraction vs. oxidative addition mechanisms for the activation of the Sâ€“H, Oâ€“H, and Câ€“H bonds using early transition metal oxides. Physical Chemistry Chemical Physics, 2021, 23, 1437-1442.	2.8	3
15	Highly Diastereoâ€•and Enantioselective Synthesis of 3,6â€²â€Bisborylâ€•anti â€1,2â€oxaborinanâ€3â€ene: An Entry to Enantioenriched Homoallylic Alcohols with A Stereodefined Trisubstituted Alkene. Angewandte Chemie - International Edition, 2021, 60, 840-848.	13.8	23
16	Electronic Structure of RhO²⁺, Its Ammoniated Complexes (NH₃)_{1â€“5}RhO²⁺, and Mechanistic Exploration of CH₄ Activation by Them. Inorganic Chemistry, 2021, 60, 16111-16119.	4.0	3
17	Aufbau Principle for Diffuse Electrons of Double-Shell Metal Ammonia Complexes: The Case of M(NH₃)₄@12NH₃, M = Li, Be⁺, B²⁺. Journal of Physical Chemistry A, 2020, 124, 505-512.	2.5	23
18	Beâ€“Be Bond in Action: Lessons from the Berylliumâ€“Ammonia Complexes [Be(NH₃)_{0â€“4}]₂^{0,2+}. Journal of Physical Chemistry A, 2020, 124, 9783-9792.	2.5	8

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19	Addressing the Hypervalent Model: A Straightforward Explanation of Traditionally Hypervalent Molecules. Journal of Chemical Education, 2020, 97, 3638-3646.	2.3	10
20	Geometric and electronic structure analysis of calcium water complexes with one and two solvation shells. Physical Chemistry Chemical Physics, 2020, 22, 22426-22435.	2.8	12
21	Isolating the Contributions of Specific Network Sites to the Diffuse Vibrational Spectrum of Interfacial Water with Isotopomer-Selective Spectroscopy of Cold Clusters. Journal of Physical Chemistry A, 2020, 124, 10393-10406.	2.5	16
22	Simultaneous Functionalization of Methane and Carbon Dioxide Mediated by Single Platinum Atomic Anions. Journal of the American Chemical Society, 2020, 142, 21556-21561.	13.7	24
23	Ab initio investigation of the ground and excited states of ZrO+ and NbO+. Journal of Quantitative Spectroscopy and Radiative Transfer, 2020, 255, 107265.	2.3	5
24	Scandium in Neutral and Positively Charged Ammonia Complexes: Balancing between Sc²⁺ and Sc³⁺. Journal of Physical Chemistry A, 2020, 124, 4400-4412.	2.5	12
25	Weak-field ligands enable inert early transition metal oxides to convert methane to methanol: the case of ZrO. Physical Chemistry Chemical Physics, 2020, 22, 6606-6618.	2.8	10
26	Ab initio investigation of the ground and excited states of RuO^{+,0,â^'} and their reaction with water. Physical Chemistry Chemical Physics, 2020, 22, 16072-16079.	2.8	10
27	Metal-Free Activation of N₂ by Persistent Carbene Pairs: An Ab Initio Investigation. Journal of Physical Chemistry C, 2019, 123, 21548-21553.	3.1	8
28	Stability and Electronic Features of Calcium Hexa-, Hepta-, and Octa-Coordinated Ammonia Complexes: A First-Principles Study. Journal of Physical Chemistry A, 2019, 123, 6744-6750.	2.5	22
29	Superatomic nature of alkaline earth metalâ€“water complexes: the cases of Be(H₂O)0,+4 and Mg(H₂O)0,+6. Physical Chemistry Chemical Physics, 2019, 21, 15861-15870.	2.8	20
30	Oâ€“H and Câ€“H Bond Activations of Water and Methane by RuO2+ and (NH3)RuO2+: Ground and Excited States. Journal of Physical Chemistry A, 2019, 123, 9336-9344.	2.5	10
31	Electronic and structural features of octa-coordinated yttriumâ€“ammonia complexes: the first neutral solvated electron precursor with eight ligands and three outer electrons. Physical Chemistry Chemical Physics, 2019, 21, 7098-7104.	2.8	17
32	Methane to Methanol Conversion Facilitated by Transition-Metal Methyl and Methoxy Units: The Cases of FeCH₃⁺ and FeOCH₃⁺. Journal of Physical Chemistry A, 2019, 123, 5590-5599.	2.5	12
33	The interaction-induced dipole of H2â€“H: Newab initioresults and spherical tensor analysis. Journal of Chemical Physics, 2019, 150, 204307.	3.0	1
34	Electronic and geometric structure analysis of neutral and anionic metal nitric chalcogens: The case of MNX series (M=Li, Na, Be and X=O, S, Se, Te). Journal of Computational Chemistry, 2019, 40, 1740-1751.	3.3	3
35	Transition-metal solvated-electron precursors: diffuse and 3d electrons in V(NH₃)0,Â±6. Physical Chemistry Chemical Physics, 2019, 21, 7090-7097.	2.8	19
36	Selective Activation of the Câ^'H Bond in Methane by Single Platinum Atomic Anions. Angewandte Chemie - International Edition, 2019, 58, 7773-7777.	13.8	27

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37	Selective Activation of the Câ^'H Bond in Methane by Single Platinum Atomic Anions. Angewandte Chemie, 2019, 131, 7855-7859.	2.0	11
38	â€œHypervalencyâ€•and the chemical bond. Computational and Theoretical Chemistry, 2019, 1153, 65-74.	2.5	11
39	Electronic and geometric structure analysis of neutral and anionic alkali metal complexes of the CX series (Xâ€‰=â€‰O, S, Se, Te, Po): The case of M(CX)_{nâ€‰=â€‰1â€“4} (Mâ€‰=â€‰Li, Na, and their dimers Journal of Computational Chemistry, 2019, 40, 1344-1351.	3.3	8
40	Carbon monoxide activation by atomic thorium: ground and excited state reaction pathways. Physical Chemistry Chemical Physics, 2019, 21, 24469-24477.	2.8	3
41	Quantum chemical calculations on NbO and its reaction with methane: ground and excited electronic states. Physical Chemistry Chemical Physics, 2019, 21, 26324-26332.	2.8	11
42	Ab initio investigation of the ground and excited states of MoO+,2+,â^' and their catalytic strength on water activation. Physical Chemistry Chemical Physics, 2018, 20, 12278-12287.	2.8	15
43	Aufbau Rules for Solvated Electron Precursors: Be(NH₃)₄^{0,Â±} Complexes and Beyond. Journal of Physical Chemistry Letters, 2018, 9, 84-88.	4.6	37
44	Ligand field effects on the ground and excited states of reactive FeO²⁺ species. Physical Chemistry Chemical Physics, 2018, 20, 28786-28795.	2.8	29
45	Dependence of the multipole moments, static polarizabilities, and static hyperpolarizabilities of the hydrogen molecule on the Hâ€“H separation in the ground singlet state. Journal of Chemical Physics, 2018, 149, 234103.	3.0	9
46	Communication: Water activation and splitting by single metal-atom anions. Journal of Chemical Physics, 2018, 149, 221101.	3.0	22
47	Enantioselective Allenylation of Aldehydes via BrÃ¸nsted Acid Catalysis. Advanced Synthesis and Catalysis, 2018, 360, 4634-4639.	4.3	47
48	Molecules mimicking atoms: monomers and dimers of alkali metal solvated electron precursors. Physical Chemistry Chemical Physics, 2018, 20, 24186-24191.	2.8	29
49	Dative bonds versus electron solvation in triâ€coordinated beryllium complexes: Be(CX)₃ [X = O, S, Se, Te, Po] and Be(PH₃)₃ versus Be(NH₃)₃. International Journal of Quantum Chemistry, 2018, 118, e25673.	2.0	16
50	Ab initio calculations on the ground and excited electronic states of neutral and charged palladium monoxide, PdO^{0,+,â^'}. Physical Chemistry Chemical Physics, 2018, 20, 14578-14586.	2.8	15
51	Enantioselective Syntheses of Homopropargylic Alcohols via Asymmetric Allenylboration. Organic Letters, 2018, 20, 3810-3814.	4.6	51
52	Th(<scp>iv</scp>) and Ce(<scp>iv</scp>) napthylsalophen sandwich complexes: characterization of unusual thorium fluorescence in solution and solid-state. Chemical Communications, 2017, 53, 11984-11987.	4.1	27
53	Ortho-para interconversion in cation-water complexes: The case of V+(H2O) and Nb+(H2O) clusters. Journal of Chemical Physics, 2017, 146, 224305.	3.0	8
54	The Versatile Personality of Beryllium: Be(O₂)_{1â€“2} vs Be(CO)_{1â€“2}. Journal of Physical Chemistry A, 2017, 121, 7051-7058.	2.5	6

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55	The role of O(¹D) in the oxidation mechanism of ethylene by iodosobenzene and other hypervalent molecules. Physical Chemistry Chemical Physics, 2017, 19, 18152-18155.	2.8	3
56	A periodic-DFT study of retro-aldol fragmentation of fuctose on MoO3. Applied Catalysis A: General, 2017, 530, 75-82.	4.3	6
57	Isotopomer-selective spectra of a single intact H2O molecule in the Cs+(D2O)5H2O isotopologue: Going beyond pattern recognition to harvest the structural information encoded in vibrational spectra. Journal of Chemical Physics, 2016, 144, 074305.	3.0	23
58	A New, Dispersion-Driven Intermolecular Arrangement for the Benzeneâ€“Water Octamer Complex: Isomers and Analysis of their Vibrational Spectra. Journal of Chemical Theory and Computation, 2016, 12, 4004-4014.	5.3	11
59	The Origin of the Reactivity of the Criegee Intermediate: Implications for Atmospheric Particle Growth. Angewandte Chemie, 2016, 128, 1027-1031.	2.0	14
60	The Origin of the Reactivity of the Criegee Intermediate: Implications for Atmospheric Particle Growth. Angewandte Chemie - International Edition, 2016, 55, 1015-1019.	13.8	36
61	On the validity of the basis set superposition error and complete basis set limit extrapolations for the binding energy of the formic acid dimer. Journal of Chemical Physics, 2015, 142, 094311.	3.0	40
62	An accurate and efficient computational protocol for obtaining the complete basis set limits of the binding energies of water clusters at the MP2 and CCSD(T) levels of theory: Application to (H2O)m, m = 2-6, 8, 11, 16, and 17. Journal of Chemical Physics, 2015, 142, 234303.	3.0	54
63	Ground and Excited States of the [Fe(H₂O)₆]²⁺ and [Fe(H₂O)₆]³⁺ Clusters: Insight into the Electronic Structure of the [Fe(H₂O)₆]²⁺â€“[Fe(H₂O)₆]³⁺ Complex. Journal of Chemical Theory and Computation, 2015, 11, 1549-1563.	5.3	22
64	Quantum mechanical calculation of the collision-induced absorption spectra of N2â€“N2 with anisotropic interactions. Journal of Chemical Physics, 2015, 142, 084306.	3.0	26
65	A new variation of the Buckingham exponential-6 potential with a tunable, singularity-free short-range repulsion and an adjustable long-range attraction. Chemical Physics Letters, 2015, 619, 133-138.	2.6	9
66	Low energy isomers of (H2O)25 from a hierarchical method based on Monte Carlo temperature basin paving and molecular tailoring approaches benchmarked by MP2 calculations. Journal of Chemical Physics, 2014, 141, 164304.	3.0	23
67	Unimolecular and hydrolysis channels for the detachment of water from microsolvated alkaline earth dication (Mg2+, Ca2+, Sr2+, Ba2+) clusters. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	11
68	Elucidating the mechanism behind the stabilization of multi-charged metal cations in water: a case study of the electronic states of microhydrated Mg2+, Ca2+ and Al3+. Physical Chemistry Chemical Physics, 2014, 16, 6886.	2.8	16
69	On the Bonding Nature of Ozone (O₃) and Its Sulfur-Substituted Analogues SO₂, OS₂, and S₃: Correlation between Their Biradical Character and Molecular Properties. Journal of the American Chemical Society, 2014, 136, 2808-2817.	13.7	66
70	Benchmark Theoretical Study of the Ï€â€“Ï€ Binding Energy in the Benzene Dimer. Journal of Physical Chemistry A, 2014, 118, 7568-7578.	2.5	77
71	Optimal geometries and harmonic vibrational frequencies of the global minima of water clusters (H2O)n, n = 2â€“6, and several hexamer local minima at the CCSD(T) level of theory. Journal of Chemical Physics, 2013, 139, 114302.	3.0	105
72	Unusual Inorganic Biradicals: A Theoretical Analysis. Angewandte Chemie - International Edition, 2013, 52, 5736-5739.	13.8	75

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73	Efficient Procedure for the Numerical Calculation of Harmonic Vibrational Frequencies Based on Internal Coordinates. Journal of Physical Chemistry A, 2013, 117, 7019-7029.	2.5	9
74	Hirshfeld density partitioning technique: A first application to the transition metal compounds, HScO, TiO, VO. Journal of Chemical Physics, 2013, 138, 184305.	3.0	5
75	Ground and excited states of vanadium hydroxide isomers and their cations, VOH0,+ and HVO0,+. Journal of Chemical Physics, 2013, 138, 114305.	3.0	2
76	Interaction-induced dipoles of hydrogen molecules colliding with helium atoms: A new ab initio dipole surface for high-temperature applications. Journal of Chemical Physics, 2012, 136, 044320.	3.0	11
77	Particle in a MÃ¶bius wire and half-integer orbital angular momentum. Physical Review A, 2011, 83, .	2.5	7
78	First-Principles Calculations of the Electronic and Geometrical Structures of Neutral [Sc,O,H] Molecules and the Monocations, ScOH^{0,+} and HScO^{0,+}. Journal of Physical Chemistry A, 2011, 115, 4436-4447.	2.5	7
79	First principles study of the ground and excited states of FeO, FeO+, and FeOâ¯. Journal of Chemical Physics, 2011, 134, 234308.	3.0	63
80	Ab initio investigation of titanium hydroxide isomers and their cations, TiOH0, + and HTiO0, +. Journal of Chemical Physics, 2011, 135, 144111.	3.0	11
81	HÃ¼ckel versus MÃ¶bius aromaticity: The particle in a cylinder versus a MÃ¶bius strip. Physical Review A, 2010, 82, .	2.5	19
82	An accurate first principles study of the geometric and electronic structure of B2, B2â¯, B3, B3â¯, and B3H: Ground and excited states. Journal of Chemical Physics, 2010, 132, 164307.	3.0	16
83	Electronic Structure and Bonding of the Early 3d-Transition Metal Diatomic Oxides and Their Ions: ScO^{0,Â±}, TiO^{0,Â±}, CrO^{0,Â±}, and MnO^{0,Â±}^{â€}. Journal of Physical Chemistry A, 2010, 114, 8536-8572.	2.5	72
84	Ab initio investigation of the electronic structure and bonding of BH, BHâ¯, and HBBH molecules. Journal of Chemical Physics, 2008, 128, 144308.	3.0	28
85	All-Electron First Principles Calculations of the Ground and Some Low-Lying Excited States of BaI. Journal of Physical Chemistry A, 2007, 111, 10002-10009.	2.5	8
86	Electronic Structure of Vanadium Oxide. Neutral and Charged Species, VO0,Â±. Journal of Physical Chemistry A, 2007, 111, 1953-1965.	2.5	65
87	Carbonyl Boron and Related Systems:â€‰ An ab Initio Study of Bâ¯X and YBâ<sup>®BY (1Î£g+), Where X = He, Ne, Ar, Kr, CO, CS, N2 and Y = Ar, Kr, CO, CS, N2. Journal of Physical Chemistry A, 2004, 108, 4335-4340.	2.5	66