Yury Minenkov

List of Publications by Year in descending order

47 papers	2,785 citations	304743 22 h-index	233421 45 g-index
49 all docs	49 docs citations	49 times ranked	4139 citing authors

#	Article	IF	Citations
1	Gas-phase thermochemistry of polycyclic aromatic hydrocarbons: an approach integrating the quantum chemistry composite scheme and reaction generator. Physical Chemistry Chemical Physics, 2022, 24, 3163-3181.	2.8	8
2	Molecular Structure of Nickel Octamethylporphyrinâ€"Rare Experimental Evidence of a Ruffling Effect in Gas Phase. International Journal of Molecular Sciences, 2022, 23, 320.	4.1	4
3	â€œIn Vitroâ€•and â€œIn Vivoâ€•Diagnostic Check for the Thermochemistry of Metalâ€"Organic Compounds. Inorganic Chemistry, 2022, 61, 10743-10755.	4.0	2
4	Ambiguities in solvation free energies from cluster-continuum quasichemical theory: lithium cation in protic and aprotic solvents. Physical Chemistry Chemical Physics, 2021, 23, 16077-16088.	2.8	10
5	Thermochemistry of 5,10,15,20-tetraphenylporphyrin. Journal of Chemical Thermodynamics, 2020, 151, 106244.	2.0	6
6	Mechanistic Insight into the Photoredox-Nickel-HAT Triple Catalyzed Arylation and Alkylation of Î±-Amino C_{sp3}â€"H Bonds. Journal of the American Chemical Society, 2020, 142, 16942-16952.	13.7	69
7	Effect of fused triphenylamine core in star-shaped donor-Ï€-acceptor molecules on their physicochemical properties and performance in bulk heterojunction organic solar cells. Dyes and Pigments, 2020, 177, 108260.	3.7	18
8	Star-shaped benzotriindole-based donor-acceptor molecules: Synthesis, properties and application in bulk heterojunction and single-material organic solar cells. Dyes and Pigments, 2020, 181, 108523.	3.7	21
9	Gas-Phase Thermochemistry of MX₃ and M₂X₆ (M = Sc, Y; X = F, Cl,) Tj ETQq1 1 0.784314 rgBT Chemistry, 2020, 59, 17084-17095.	4.0	6
10	A Robust and Costâ€Efficient Scheme for Accurate Conformational Energies of Organic Molecules. ChemPhysChem, 2019, 20, 92-102.	2.1	27
11	Evaluation of experimental alkali metal ionâ€"ligand noncovalent bond strengths with DLPNO-CCSD(T) method. Journal of Chemical Physics, 2019, 151, 014301.	3.0	8
12	Gas Phase Silver Thermochemistry from First Principles. Inorganic Chemistry, 2019, 58, 7873-7885.	4.0	10
13	Structural and Energetic Impact of Nonâ€natural 7â€Deazaâ€8â€azaguanine, 7â€Deazaâ€8â€azaisoguanine, and Their 7â€Substituted Derivatives on Hydrogenâ€Bond Pairing with Cytosine and Isocytosine. ChemBioChem, 2019, 20, 2262-2270.	2.6	4
14	Unprecedented Diastereoselective Arylogous Michael Addition of Unactivated Phthalides. Chemistry - A European Journal, 2019, 25, 7043-7043.	3.3	0
15	Unprecedented Diastereoselective Arylogous Michael Addition of Unactivated Phthalides. Chemistry - A European Journal, 2019, 25, 7131-7141.	3.3	7
16	Ligand-Controlled Chemoselective C(acyl)â€"O Bond vs C(aryl)â€"C Bond Activation of Aromatic Esters in Nickel Catalyzed C(sp²)â€"C(sp³) Cross-Couplings. Journal of the American Chemical Society, 2018, 140, 3724-3735.	13.7	154
17	A Silica-Supported Monoalkylated Tungsten Dioxo Complex Catalyst for Olefin Metathesis. ACS Catalysis, 2018, 8, 2715-2729.	11.2	38
18	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.	3.0	402

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19	Insights into the Catalytic Activity of [Pd(NHC)(cin)Cl] (NHC=IPr, IPr^{Cl}, IPr^{Br}) Complexes in the Suzukiâ€“Miyaura Reaction. ChemCatChem, 2018, 10, 601-611.	3.7	21
20	Application of Semiempirical Methods to Transition Metal Complexes: Fast Results but Hard-to-Predict Accuracy. Journal of Chemical Theory and Computation, 2018, 14, 3428-3439.	5.3	36
21	Metathetic Oxidation of 2-Butenes to Acetaldehyde by Molecular Oxygen Using the Single-Site Olefin Metathesis Catalyst (â‰¡SiO)₂Mo(â•O)₂. ACS Catalysis, 2018, 8, 7549-7555.	11.2	21
22	Accurate Gas Phase Formation Enthalpies of Alloys and Refractories Decomposition Products. Inorganic Chemistry, 2017, 56, 1386-1401.	4.0	17
23	Pair natural orbital and canonical coupled cluster reaction enthalpies involving light to heavy alkali and alkaline earth metals: the importance of sub-valence correlation. Physical Chemistry Chemical Physics, 2017, 19, 9374-9391.	2.8	43
24	Switchable Diastereoselectivity in the Fluoride-Promoted Vinylogous Mukaiyamaâ€“Michael Reaction of 2-[(Trimethylsilyl)oxy]furan Catalyzed by Crown Ethers. Journal of Organic Chemistry, 2017, 82, 6629-6637.	3.2	9
25	Well-Defined Silica Grafted Molybdenum Bis(imido) Catalysts for Imine Metathesis Reactions. Organometallics, 2017, 36, 1550-1556.	2.3	12
26	Accurate experimental and theoretical enthalpies of association of TiCl₄ with typical Lewis bases used in heterogeneous Zieglerâ€“Natta catalysis. Physical Chemistry Chemical Physics, 2017, 19, 26996-27006.	2.8	30
27	Ground-State Gas-Phase Structures of Inorganic Molecules Predicted by Density Functional Theory Methods. ACS Omega, 2017, 2, 8373-8387.	3.5	14
28	Heats of Formation of Medium-Sized Organic Compounds from Contemporary Electronic Structure Methods. Journal of Chemical Theory and Computation, 2017, 13, 3537-3560.	5.3	45
29	Treating Subvalence Correlation Effects in Domain Based Pair Natural Orbital Coupled Cluster Calculations: An Out-of-the-Box Approach. Journal of Chemical Theory and Computation, 2017, 13, 3220-3227.	5.3	45
30	Catalytic Î±-Arylation of Imines Leading to N-Unprotected Indoles and Azaindoles. ACS Catalysis, 2016, 6, 2930-2938.	11.2	26
31	Troubles in the Systematic Prediction of Transition Metal Thermochemistry with Contemporary Out-of-the-Box Methods. Journal of Chemical Theory and Computation, 2016, 12, 1542-1560.	5.3	42
32	Tungsten(VI) Carbyne/Bis(carbene) Tautomerization Enabled by Nâ€Đonor SBA15 Surface Ligands: A Solidâ€State NMR and DFT Study. Angewandte Chemie - International Edition, 2016, 55, 11162-11166.	13.8	13
33	Controlling the hydrogenolysis of silica-supported tungsten pentamethyl leads to a class of highly electron deficient partially alkylated metal hydrides. Chemical Science, 2016, 7, 1558-1568.	7.4	53
34	Cooperative Effect of Monopodal Silica-Supported Niobium Complex Pairs Enhancing Catalytic Cyclic Carbonate Production. Journal of the American Chemical Society, 2015, 137, 7728-7739.	13.7	123
35	N-heterocyclic carbene copper(<scp>i</scp>) catalysed N-methylation of amines using CO₂. Dalton Transactions, 2015, 44, 18138-18144.	3.3	81
36	Accuracy of DLPNOâ€“CCSD(T) Method for Noncovalent Bond Dissociation Enthalpies from Coinage Metal Cation Complexes. Journal of Chemical Theory and Computation, 2015, 11, 4664-4676.	5.3	85

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37	A Highly Selective Copperâ€“Indium Bimetallic Electrocatalyst for the Electrochemical Reduction of Aqueous CO₂ to CO. Angewandte Chemie - International Edition, 2015, 54, 2146-2150.	13.8	403
38	Complete Reaction Pathway of Ruthenium-Catalyzed Olefin Metathesis of Ethyl Vinyl Ether: Kinetics and Mechanistic Insight from DFT. Organometallics, 2013, 32, 2099-2111.	2.3	71
39	The accuracy of DFT-optimized geometries of functional transition metal compounds: a validation study of catalysts for olefin metathesis and other reactions in the homogeneous phase. Dalton Transactions, 2012, 41, 5526.	3.3	429
40	Molecular structure and bonding in octamethylporphyrin tin(ii), SnN4C28H28. Dalton Transactions, 2012, 41, 7550.	3.3	23
41	The Nature of the Barrier to Phosphane Dissociation from Grubbs Olefin Metathesis Catalysts. European Journal of Inorganic Chemistry, 2012, 2012, 1507-1516.	2.0	38
42	Thermodynamic and kinetic characteristics of liquid phase hydrogenation of substituted nitrobenzenes. Russian Journal of Physical Chemistry A, 2012, 86, 908-912.	0.6	0
43	Neutral Nickel Oligoâ€•and Polymerization Catalysts: The Importance of Alkyl Phosphine Intermediates in Chain Termination. Chemistry - A European Journal, 2011, 17, 14628-14642.	3.3	16
44	Octamethylporphyrin copper, C28H28N4Cu â€“ A first experimental structure determination of porphyrins in gas phase. Journal of Molecular Structure, 2010, 978, 163-169.	3.6	16
45	On the nature of the active site in ruthenium olefin coordinationâ€“insertion polymerization catalystsâ˜†. Journal of Molecular Catalysis A, 2010, 324, 64-74.	4.8	8
46	Metalâ^'Phosphine Bond Strengths of the Transition Metals: A Challenge for DFT. Journal of Physical Chemistry A, 2009, 113, 11833-11844.	2.5	127
47	16OSTM10: A new open-shell transition metal conformational energies database to challenge contemporary semiempirical and force field methods. Physical Chemistry Chemical Physics, 0, , .	2.8	5