

Timofei Privalov

List of Publications by Year in descending order

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64
papers

3,594
citations

159585

30
h-index

133252

59
g-index

68
all docs

68
docs citations

68
times ranked

3670
citing authors

#	ARTICLE	IF	CITATIONS
1	A molecular ruthenium catalyst with water-oxidation activity comparable to that of photosystem II. <i>Nature Chemistry</i> , 2012, 4, 418-423.	13.6	1,131
2	Structural Modifications of Mononuclear Ruthenium Complexes: A Combined Experimental and Theoretical Study on the Kinetics of Ruthenium-Catalyzed Water Oxidation. <i>Angewandte Chemie - International Edition</i> , 2011, 50, 445-449.	13.8	177
3	Evolution of O ₂ in a Seven-Coordinate Ru ^{IV} Dimer Complex with a [HOHOH] ⁺ Bridge: A Computational Study. <i>Angewandte Chemie - International Edition</i> , 2010, 49, 1773-1777.	13.8	155
4	Using Mechanistic and Computational Studies To Explain Ligand Effects in the Palladium-Catalyzed Aerobic Oxidation of Alcohols. <i>Journal of the American Chemical Society</i> , 2005, 127, 8499-8507.	13.7	127
5	Mechanistic Study of Hydrogen Transfer to Imines from a Hydroxycyclopentadienyl Ruthenium Hydride. Experimental Support for a Mechanism Involving Coordination of Imine to Ruthenium Prior to Hydrogen Transfer. <i>Journal of the American Chemical Society</i> , 2006, 128, 14293-14305.	13.7	125
6	A Study of the Interactions between Ir ^{III} /I ^{III} Redox Mediators and Organometallic Sensitizing Dyes in Solar Cells. <i>Journal of Physical Chemistry C</i> , 2009, 113, 783-790.	3.1	101
7	Toward Controlling Water Oxidation Catalysis: Tunable Activity of Ruthenium Complexes with Axial Imidazole/DMSO Ligands. <i>Journal of the American Chemical Society</i> , 2012, 134, 18868-18880.	13.7	101
8	Water Oxidation by Single-Site Ruthenium Complexes: Using Ligands as Redox and Proton Transfer Mediators. <i>Angewandte Chemie - International Edition</i> , 2012, 51, 11589-11593.	13.8	94
9	Duration of x-ray Raman scattering. <i>Physical Review A</i> , 1999, 59, 380-389.	2.5	91
10	The Importance of Alkali Cations in the [RuCl ₂ (p-cymene)] ₂ Pseudo-dipeptide-Catalyzed Enantioselective Transfer Hydrogenation of Ketones. <i>Chemistry - A European Journal</i> , 2006, 12, 3218-3225.	3.3	69
11	The Mechanism of Water Exchange in AmO ₂ (H ₂ O) ₅ ²⁺ and in the Isoelectronic UO ₂ (H ₂ O) ₅ ²⁺ and NpO ₂ (H ₂ O) ₅ ²⁺ Complexes as Studied by Quantum Chemical Methods. <i>Journal of the American Chemical Society</i> , 2004, 126, 7766-7767.	13.7	63
12	Collapse of vibrational structure in spectra of resonant x-ray Raman scattering. <i>Physical Review A</i> , 1997, 56, 256-264.	2.5	61
13	Theoretical Studies of the Mechanism of Aerobic Alcohol Oxidation with Palladium Catalyst Systems. <i>Organometallics</i> , 2005, 24, 885-893.	2.3	57
14	On the validity of the equivalent cores approximation for computing X-ray photoemission and photoabsorption spectral bands. <i>Chemical Physics</i> , 2000, 260, 11-28.	1.9	56
15	A Computational Study of O-O Bond Formation Catalyzed by Mono- and Bis-Mn ^{IV} Corrole Complexes. <i>Inorganic Chemistry</i> , 2007, 46, 7075-7086.	4.0	56
16	DFT Study of an Inner-Sphere Mechanism in the Hydrogen Transfer from a Hydroxycyclopentadienyl Ruthenium Hydride to Imines. <i>Organometallics</i> , 2007, 26, 2840-2848.	2.3	55
17	A Theoretical Study of the Essential Role of DMSO as a Solvent/Ligand in the Pd(OAc) ₂ /DMSO Catalyst System for Aerobic Oxidation. <i>Organometallics</i> , 2005, 24, 6019-6028.	2.3	52
18	Structure and Thermodynamics of Uranium(VI) Complexes in the Gas Phase: A Comparison of Experimental and ab Initio Data. <i>Journal of Physical Chemistry A</i> , 2002, 106, 11277-11282.	2.5	49

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19	On the possibility of catalytic reduction of carbonyl moieties with tris(pentafluorophenyl)borane and H ₂ : a computational study. Dalton Transactions, 2009, , 5780.	3.3	49
20	On the Possibility of Conversion of Alcohols to Ketones and Aldehydes by Phosphinoboranes R ₂ PBR ₂ : A Computational Study. Chemistry - A European Journal, 2009, 15, 1825-1829.	3.3	48
21	Aerobic Oxidation of 1-Phenylethanol Catalyzed by Palladaheterocycles. Advanced Synthesis and Catalysis, 2004, 346, 237-244.	4.3	42
22	The O-H Bonding in Water Oxidation: the Electronic Structure Portrayal of a Concerted Oxygen Atom-Proton Transfer Pathway. Chemistry - A European Journal, 2011, 17, 8313-8317.	3.3	40
23	Hydrogenation of imines by phosphonium borate zwitterions: a theoretical study. Dalton Transactions, 2009, , 1321.	3.3	39
24	The Role of Amine-B(C ₆ F ₅) ₃ Adducts in the Catalytic Reduction of Imines with H ₂ : A Computational Study. European Journal of Inorganic Chemistry, 2009, 2009, 2229-2237.	2.0	38
25	Regeneration of Oxidized Organic Photosensitizers in Grätzel Solar Cells: Quantum-Chemical Portrait of a General Mechanism. ChemPhysChem, 2010, 11, 1858-1862.	2.1	38
26	Electron Transfer in Uranyl(VI)-Uranyl(V) Complexes in Solution. Journal of the American Chemical Society, 2004, 126, 9801-9808.	13.7	37
27	Racemization of Alcohols Catalyzed by [RuCl(CO) ₂ (1-pentaphenylcyclopentadienyl)] Mechanistic Insights from Theoretical Modeling. Chemistry - A European Journal, 2009, 15, 5220-5229.	3.3	36
28	Self-Adaptable Catalysts: Substrate-Dependent Ligand Configuration. Journal of the American Chemical Society, 2008, 130, 1845-1855.	13.7	34
29	Conformational Preferences and Enantiodiscrimination of Phosphino-4-(1-hydroxyalkyl)oxazoline-Metal-Olefin Complexes Resulting from an OH-Metal Hydrogen Bond. Journal of Organic Chemistry, 2005, 70, 9882-9891.	3.2	32
30	Ab initio dynamics trajectory study of the heterolytic cleavage of H ₂ by a Lewis acid [B(C ₆ F ₅) ₃] and a Lewis base [P(tBu) ₃]. Journal of Chemical Physics, 2013, 138, 154305.	3.0	30
31	Frustation of Orbital Interactions in Lewis Base/Lewis Acid Adducts: A Computational Study of H ₂ Uptake by Phosphanylboranes R ₂ P=BR ₂ . European Journal of Inorganic Chemistry, 2009, 2009, 2759-2764.	2.0	28
32	CO Assistance in Ligand Exchange of a Ruthenium Racemization Catalyst: Identification of an Acyl Intermediate. Journal of the American Chemical Society, 2009, 131, 9500-9501.	13.7	27
33	Reduction of Uranyl(VI) by Iron(II) in Solutions: An Ab Initio Study. Journal of Physical Chemistry A, 2003, 107, 587-592.	2.5	24
34	Uncovering the Role of Intra- and Intermolecular Motion in Frustrated Lewis Acid/Base Chemistry: Ab Initio Molecular Dynamics Study of CO ₂ Binding by Phosphorus/Boron Frustrated Lewis Pair [tBu ₃ P/B(C ₆ F ₅) ₃]. Inorganic Chemistry, 2014, 53, 4598-4609.	4.0	23
35	Ab Initio Molecular Dynamics with Explicit Solvent Reveals a Two-Step Pathway in the Frustrated Lewis Pair Reaction. Chemistry - A European Journal, 2015, 21, 17708-17720.	3.3	22
36	Ab Initio Studies of Np and Pu Complexes and Reactions in the Gas Phase: Structures and Thermodynamics. Journal of Physical Chemistry A, 2003, 107, 9705-9711.	2.5	21

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37	How Frustrated Lewis Acid/Base Systems Pass through Transition- σ -State Regions: H_2 Cleavage by $[t\text{-Bu}_3\text{P}(\text{C}_6\text{F}_5)_3]_3$. ChemPhysChem, 2014, 15, 2936-2944.	2.1	21
38	A computational study of the CO dissociation in cyclopentadienyl ruthenium complexes relevant to the racemization of alcohols. Dalton Transactions, 2013, 42, 927-934.	3.3	19
39	Chemistry of Intermolecular Frustrated Lewis Pairs in Motion: Emerging Perspectives and Prospects. Israel Journal of Chemistry, 2015, 55, 179-195.	2.3	19
40	Ab Initio Molecular Dynamics Study of Hydrogen Cleavage by a Lewis Base $[t\text{-Bu}_3\text{P}]$ and a Lewis Acid $[\text{B}(\text{C}_6\text{F}_5)_3]$ at the Mesoscopic Level- σ Dynamics in the Solute- σ Solvent Molecular Clusters. ChemPhysChem, 2014, 15, 3714-3719.	2.1	16
41	Carbonyl Activation by Borane Lewis Acid Complexation: Transition States of H_2 Splitting at the Activated Carbonyl Carbon Atom in a Lewis Basic Solvent and the Proton-Transfer Dynamics of the Boroalkoxide Intermediate. Chemistry - A European Journal, 2017, 23, 9098-9113.	3.3	16
42	H_2 Cleavage by Frustrated Lewis Pairs Characterized by the Energy Decomposition Analysis of Transition States: An Alternative to the Electron Transfer and Electric Field Models. Journal of Physical Chemistry A, 2018, 122, 7202-7211.	2.5	16
43	Oxidation of Ethers, Alcohols, and Unfunctionalized Hydrocarbons by the Methyltrioxorhenium/ H_2O_2 System: A Computational Study on Catalytic $C-H$ Bond Activation. Chemistry - A European Journal, 2009, 15, 1862-1869.	3.3	15
44	Spin-Orbit Effects in Electron Transfer in Neptunyl(VI)-Neptunyl(V) Complexes in Solution. Journal of Physical Chemistry A, 2005, 109, 4957-4960.	2.5	14
45	A Prediction of Proton-Catalyzed Hydrogenation of Ketones in Lewis Basic Solvent through Facile Splitting of Hydrogen Molecules. Chemistry - A European Journal, 2017, 23, 1036-1039.	3.3	13
46	Mechanisms of Ligand Exchange Reactions, A Quantum Chemical Study of the Reaction $UO_2^{2+}(\text{Aq}) + \text{HF}(\text{Aq}) \rightarrow UO_2\text{F}^+(\text{Aq}) + \text{H}^+(\text{Aq})$. Journal of Physical Chemistry A, 2003, 107, 9456-9462.	2.5	12
47	Electron Transfer in Neptunyl(VI)-Neptunyl(V) Complexes in Solution. Journal of Physical Chemistry A, 2005, 109, 4950-4956.	2.5	11
48	Role of electron-phonon interaction in resonant x-ray Raman scattering by polymers and solids. Physical Review B, 1999, 59, 9243-9258.	3.2	10
49	X-Ray absorption and photoionization of laser excited molecules. Journal of Electron Spectroscopy and Related Phenomena, 2003, 129, 43-54.	1.7	9
50	Liberation of H_2 from $(\text{C}_6\text{H}_4\text{Me})_3\text{P}^+\text{H}^+ + (\text{B}(\text{C}_6\text{F}_4\text{H})_3)$ ion-pair: A transition-state in the minimum energy path σ versus σ the transient species in Born-Oppenheimer molecular dynamics. Journal of Chemical Physics, 2017, 147, 014303.	3.0	7
51	Computational Elucidation of a Role That Brønsted Acidification of the Lewis Acid-Bound Water Might Play in the Hydrogenation of Carbonyl Compounds with H_2 in Lewis Basic Solvents. Chemistry - A European Journal, 2017, 23, 11489-11493.	3.3	7
52	Structurally Flexible Oxocarbenium/Borohydride Ion Pair: Dynamics of Hydride Transfer on the Background of Conformational Roaming. Journal of Physical Chemistry A, 2018, 122, 5098-5106.	2.5	7
53	Binding of CO_2 by a $\text{Mes}_2\text{PCH}_2\text{CH}_2\text{B}(\text{C}_6\text{F}_5)_2$ Species: An Involvement of the Ground State Species in a Low-Energy Pathway. Chemistry - A European Journal, 2013, 19, 16512-16517.	3.3	6
54	Multiple-pathways of carbon dioxide binding by a Lewis acid $[\text{B}(\text{C}_6\text{F}_5)_3]$ and a Lewis base $[\text{P}(\text{tBu})_3]$: The energy landscape perspective. International Journal of Quantum Chemistry, 2014, 114, 289-294.	2.0	6

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55	Testing the nature of reaction coordinate describing interaction of H ₂ with carbonyl carbon, activated by Lewis acid complexation, and the Lewis basic solvent: A Born-Oppenheimer molecular dynamics study with explicit solvent. <i>Journal of Chemical Physics</i> , 2017, 147, 094302.	3.0	6
56	Surprisingly Flexible Oxonium/Borohydride Ion Pair Configurations. <i>Journal of Physical Chemistry A</i> , 2018, 122, 3713-3727.	2.5	6
57	Soft and hard x-ray Raman scattering by oriented symmetrical molecules: Selection rules, interference, and dephasing mechanisms. <i>Journal of Chemical Physics</i> , 1998, 109, 5060-5069.	3.0	5
58	Doppler effect for bound nuclear motion and its manifestation in resonant photoemission of oriented systems. <i>Chemical Physics Letters</i> , 2000, 328, 425-430.	2.6	5
59	Continuum modeling of multi-mode vibronic excitations in near-edge x-ray absorption fine structure spectra. <i>Journal of Chemical Physics</i> , 2000, 113, 3734-3740.	3.0	5
60	Temperature dependence and Debye-Waller factors for resonant x-ray Raman scattering in solids. <i>Physical Review B</i> , 2000, 62, 13996-14005.	3.2	4
61	Theory-Based Extension of the Catalyst Scope in the Base-Catalyzed Hydrogenation of Ketones: RCOOH-Catalyzed Hydrogenation of Carbonyl Compounds with H ₂ Involving a Proton Shuttle. <i>Chemistry - A European Journal</i> , 2017, 23, 18193-18202.	3.3	4
62	Water and a Borohydride/Hydronium Intermediate in the Borane-Catalyzed Hydrogenation of Carbonyl Compounds with H ₂ in Wet Ether: A Computational Study. <i>Journal of Physical Chemistry B</i> , 2018, 122, 8952-8962.	2.6	4
63	Hydrogenation of carbon-heteroatom unsaturated bonds: An assessment of consistency of density functional methods. <i>Journal of Molecular Catalysis A</i> , 2010, 324, 97-103.	4.8	3
64	The Importance of Alkali Cations in the [RuCl ₂ (p-cymene)] ₂ -Pseudo-dipeptide-Catalyzed Enantioselective Transfer Hydrogenation of Ketones. <i>Chemistry - A European Journal</i> , 2006, 12, 6190-6190.	3.3	1