Timofei Privalov

List of Publications by Year in descending order

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	Surprisingly Flexible Oxonium/Borohydride Ion Pair Configurations. Journal of Physical Chemistry A, 2018, 122, 3713-3727.	2.5	6
2	Water and a Borohydride/Hydronium Intermediate in the Borane-Catalyzed Hydrogenation of Carbonyl Compounds with H2 in Wet Ether: A Computational Study. Journal of Physical Chemistry B, 2018, 122, 8952-8962.	2.6	4
3	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
4	H₂ 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
5	Carbonyl Activation by Borane Lewis Acid Complexation: Transition States of H₂ Splitting at the Activated Carbonyl Carbon Atom in a Lewis Basic Solvent and the Protonâ€Transfer Dynamics of the Boroalkoxide Intermediate. Chemistry - A European Journal, 2017, 23, 9098-9113.	3.3	16
6	Theoryâ€Based Extension of the Catalyst Scope in the Baseâ€Catalyzed Hydrogenation of Ketones: RCOOHâ€Catalyzed Hydrogenation of Carbonyl Compounds with H₂ Involving a Proton Shuttle. Chemistry - A European Journal, 2017, 23, 18193-18202.	3.3	4
7	Testing the nature of reaction coordinate describing interaction of H2 with carbonyl carbon, activated by Lewis acid complexation, and the Lewis basic solvent: A Born-Oppenheimer molecular dynamics study with explicit solvent. Journal of Chemical Physics, 2017, 147, 094302.	3.0	6
8	Liberation of H2 from (o-C6H4Me)3Pâ€”H(+) + (âˆ’)Hâ€”B(p-C6F4H)3 ion-pair: A transition-state in the minimum energy path versus the transient species in Born-Oppenheimer molecular dynamics. Journal of Chemical Physics, 2017, 147, 014303.	3.0	7
9	Computational Elucidation of a Role That BrÃ¸nsted Acidification of the Lewis Acidâ€Bound Water Might Play in the Hydrogenation of Carbonyl Compounds with H₂ in Lewis Basic Solvents. Chemistry - A European Journal, 2017, 23, 11489-11493.	3.3	7
10	A Prediction of Protonâ€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
11	Ab Initio Molecular Dynamics with Explicit Solvent Reveals a Twoâ€Step Pathway in the Frustrated Lewis Pair Reaction. Chemistry - A European Journal, 2015, 21, 17708-17720.	3.3	22
12	Chemistry of Intermolecular Frustrated Lewis Pairs in Motion: Emerging Perspectives and Prospects. Israel Journal of Chemistry, 2015, 55, 179-195.	2.3	19
13	Ab Initio Molecular Dynamics Study of Hydrogen Cleavage by a Lewis Base [tBu₃P] and a Lewis Acid [B(C₆F₅)₃] at the Mesoscopic Levelâ€”Dynamics in the Soluteâ€“Solvent Molecular Clusters. ChemPhysChem, 2014, 15, 3714-3719.	2.1	16
14	Multiple-pathways of carbon dioxide binding by a Lewis acid [B(C6F5)3] and a lewis base [P(tBu)3]: The energy landscape perspective. International Journal of Quantum Chemistry, 2014, 114, 289-294.	2.0	6
15	How Frustrated Lewis Acid/Base Systems Pass through Transitionâ€State Regions: H₂ Cleavage by [tBu₃P/B(C₆F₅)₃]. ChemPhysChem, 2014, 15, 2936-2944.	2.1	21
16	Uncovering the Role of Intra- and Intermolecular Motion in Frustrated Lewis Acid/Base Chemistry: Ab Initio Molecular Dynamics Study of CO₂ Binding by Phosphorus/Boron Frustrated Lewis Pair [tBu₃P/B(C₆F₅)₃]. Inorganic Chemistry, 2014, 53, 4598-4609.	4.0	23
17	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
18	Ab initio dynamics trajectory study of the heterolytic cleavage of H2 by a Lewis acid [B(C6F5)3] and a Lewis base [P(tBu)3]. Journal of Chemical Physics, 2013, 138, 154305.	3.0	30

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19	Binding of CO₂ by a Mes₂PCH₂CH₂B(C₆F₅)₂ Species: An Involvement of the Ground State Species in a Lowâ€Energy Pathway. Chemistry - A European Journal, 2013, 19, 16512-16517.	3.3	6
20	Water Oxidation by Singleâ€Site Ruthenium Complexes: Using Ligands as Redox and Proton Transfer Mediators. Angewandte Chemie - International Edition, 2012, 51, 11589-11593.	13.8	94
21	Toward Controlling Water Oxidation Catalysis: Tunable Activity of Ruthenium Complexes with Axial Imidazole/DMSO Ligands. Journal of the American Chemical Society, 2012, 134, 18868-18880.	13.7	101
22	A molecular ruthenium catalyst with water-oxidation activity comparable to that of photosystem II. Nature Chemistry, 2012, 4, 418-423.	13.6	1,131
23	Structural Modifications of Mononuclear Ruthenium Complexes:â€… A Combined Experimental and Theoretical Study on the Kinetics of Rutheniumâ€Catalyzed Water Oxidation. Angewandte Chemie - International Edition, 2011, 50, 445-449.	13.8	177
24	The Oï£¿O Bonding in Water Oxidation: the Electronic Structure Portrayal of a Concerted Oxygen Atomâ€“Proton Transfer Pathway. Chemistry - A European Journal, 2011, 17, 8313-8317.	3.3	40
25	Regeneration of Oxidized Organic Photoâ€Sensitizers in GrÃtzel Solar Cells: Quantumâ€Chemical Portrait of a General Mechanism. ChemPhysChem, 2010, 11, 1858-1862.	2.1	38
26	Evolution of O₂ in a Sevenâ€Coordinate Ru^{IV} Dimer Complex with a [HOHOH]^{â¯} Bridge: A Computational Study. Angewandte Chemie - International Edition, 2010, 49, 1773-1777.	13.8	155
27	Hydrogenation of carbon-heteroatom unsaturated bonds: An assessment of consistency of density functional methodsâ¯†. Journal of Molecular Catalysis A, 2010, 324, 97-103.	4.8	3
28	Oxidation of Ethers, Alcohols, and Unfunctionalized Hydrocarbons by the Methyltrioxorhenium/H₂O₂ System: A Computational Study on Catalytic Cï£¿H Bond Activation. Chemistry - A European Journal, 2009, 15, 1862-1869.	3.3	15
29	On the Possibility of Conversion of Alcohols to Ketones and Aldehydes by Phosphinoboranes R₂PBRâ€²Râ€²â€²: A Computational Study. Chemistry - A European Journal, 2009, 15, 1825-1829.	3.3	48
30	Racemization of Alcohols Catalyzed by [RuCl(CO)₂(Î·⁵â€pentaphenylcyclopentadienyl)]â€”Mechanistic Insights from Theoretical Modeling. Chemistry - A European Journal, 2009, 15, 5220-5229.	3.3	36
31	The Role of Amineâ€“B(C₆F₅)₃ Adducts in the Catalytic Reduction of Imines with H₂: A Computational Study. European Journal of Inorganic Chemistry, 2009, 2009, 2229-2237.	2.0	38
32	â€œFrustrationâ€•of Orbital Interactions in Lewis Base/Lewis Acid Adducts: A Computational Study of H2Uptake by Phosphanylboranes R2P=BRâ€²2. European Journal of Inorganic Chemistry, 2009, 2009, 2759-2764.	2.0	28
33	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
34	A Study of the Interactions between Iâ¯/I3â¯ Redox Mediators and Organometallic Sensitizing Dyes in Solar Cells. Journal of Physical Chemistry C, 2009, 113, 783-790.	3.1	101
35	On the possibility of catalytic reduction of carbonyl moieties with tris(pentafluorophenyl)borane and H2: a computational study. Dalton Transactions, 2009, , 5780.	3.3	49
36	Hydrogenation of imines by phosphonium borate zwitterions: a theoretical study. Dalton Transactions, 2009, , 1321.	3.3	39

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37	Self-Adaptable Catalysts:â€‰ Substrate-Dependent Ligand Configuration. Journal of the American Chemical Society, 2008, 130, 1845-1855.	13.7	34
38	DFT Study of an Inner-Sphere Mechanism in the Hydrogen Transfer from a Hydroxycyclopentadienyl Ruthenium Hydride to Imines. Organometallics, 2007, 26, 2840-2848.	2.3	55
39	A Computational Study of Oâ^'O Bond Formation Catalyzed by Mono- and Bis-MnIVâ^'Corrole Complexes. Inorganic Chemistry, 2007, 46, 7075-7086.	4.0	56
40	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. Journal of the American Chemical Society, 2006, 128, 14293-14305.	13.7	125
41	The Importance of Alkali Cations in the [{RuCl2(p-cymene)}2]â€“Pseudo-dipeptide-Catalyzed Enantioselective Transfer Hydrogenation of Ketones. Chemistry - A European Journal, 2006, 12, 3218-3225.	3.3	69
42	The Importance of Alkali Cations in the [{RuCl2(p-cymene)}2]â€“Pseudo-dipeptide-Catalyzed Enantioselective Transfer Hydrogenation of Ketones. Chemistry - A European Journal, 2006, 12, 6190-6190.	3.3	1
43	Using Mechanistic and Computational Studies To Explain Ligand Effects in the Palladium-Catalyzed Aerobic Oxidation of Alcohols. Journal of the American Chemical Society, 2005, 127, 8499-8507.	13.7	127
44	Electron Transfer in Neptunyl(VI)â^'Neptunyl(V) Complexes in Solution. Journal of Physical Chemistry A, 2005, 109, 4950-4956.	2.5	11
45	A Theoretical Study of the Essential Role of DMSO as a Solvent/Ligand in the Pd(OAc)2/DMSO Catalyst System for Aerobic Oxidation. Organometallics, 2005, 24, 6019-6028.	2.3	52
46	Conformational Preferences and Enantiodiscrimination of Phosphino-4-(1-hydroxyalkyl)oxazolineâ^'Metalâ^'Olefin Complexes Resulting from an OHâ^'Metal Hydrogen Bond. Journal of Organic Chemistry, 2005, 70, 9882-9891.	3.2	32
47	Spinâ^'Orbit Effects in Electron Transfer in Neptunyl(VI)â^'Neptunyl(V) Complexes in Solution. Journal of Physical Chemistry A, 2005, 109, 4957-4960.	2.5	14
48	Theoretical Studies of the Mechanism of Aerobic Alcohol Oxidation with Palladium Catalyst Systems. Organometallics, 2005, 24, 885-893.	2.3	57
49	The Mechanism of Water Exchange in AmO2(H2O)52+ and in the Isoelectronic UO2(H2O)5+ and NpO2(H2O)52+ Complexes as Studied by Quantum Chemical Methods. Journal of the American Chemical Society, 2004, 126, 7766-7767.	13.7	63
50	Aerobic Oxidation of 1-Phenylethanol Catalyzed by Palladaheterocycles. Advanced Synthesis and Catalysis, 2004, 346, 237-244.	4.3	42
51	Electron Transfer in Uranyl(VI)â^'Uranyl(V) Complexes in Solution. Journal of the American Chemical Society, 2004, 126, 9801-9808.	13.7	37
52	Ab Initio Studies of Np and Pu Complexes and Reactions in the Gas Phase:â€‰ Structures and Thermodynamics. Journal of Physical Chemistry A, 2003, 107, 9705-9711.	2.5	21
53	X-Ray absorption and photoionization of laser excited molecules. Journal of Electron Spectroscopy and Related Phenomena, 2003, 129, 43-54.	1.7	9
54	Reduction of Uranyl(VI) by Iron(II) in Solutions:â€‰ An Ab Initio Study. Journal of Physical Chemistry A, 2003, 107, 587-592.	2.5	24

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55	Mechanisms of Ligand Exchange Reactions, A Quantum Chemical Study of the Reaction UO22+(Aq) + HF(Aq) â†' UO2F+(Aq) + H+(Aq). Journal of Physical Chemistry A, 2003, 107, 9456-9462.	2.5	12
56	Structure and Thermodynamics of Uranium(VI) Complexes in the Gas Phase: A Comparison of Experimental and ab Initio Data. Journal of Physical Chemistry A, 2002, 106, 11277-11282.	2.5	49
57	Doppler effect for bound nuclear motion and its manifestation in resonant photoemission of oriented systems. Chemical Physics Letters, 2000, 328, 425-430.	2.6	5
58	On the validity of the equivalent cores approximation for computing X-ray photoemission and photoabsorption spectral bands. Chemical Physics, 2000, 260, 11-28.	1.9	56
59	Continuum modeling of multi-mode vibronic excitations in near-edge x-ray absorption fine structure spectra. Journal of Chemical Physics, 2000, 113, 3734-3740.	3.0	5
60	Temperature dependence and Debye-Waller factors for resonant x-ray Raman scattering in solids. Physical Review B, 2000, 62, 13996-14005.	3.2	4
61	Duration of x-ray Raman scattering. Physical Review A, 1999, 59, 380-389.	2.5	91
62	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
63	Soft and hard x-ray Raman scattering by oriented symmetrical molecules: Selection rules, interference, and dephasing mechanisms. Journal of Chemical Physics, 1998, 109, 5060-5069.	3.0	5
64	Collapse of vibrational structure in spectra of resonant x-ray Raman scattering. Physical Review A, 1997, 56, 256-264.	2.5	61