Elena Jakubikova

List of Publications by Year
in descending order

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56 papers	1,773 citations	331670 21 h-index	276875 41 g-index
58 all docs	58 docs citations	58 times ranked	2336 citing authors

#	Article	IF	Citations
1	Calculation of One-Electron Redox Potentials Revisited. Is It Possible to Calculate Accurate Potentials with Density Functional Methods?. Journal of Physical Chemistry A, 2009, 113, 6745-6750.	2.5	270
2	Low-Spin versus High-Spin Ground State in Pseudo-Octahedral Iron Complexes. Inorganic Chemistry, 2012, 51, 6011-6019.	4.0	116
3	Ironing out the photochemical and spin-crossover behavior of Fe(II) coordination compounds with computational chemistry. Coordination Chemistry Reviews, 2017, 337, 97-111.	18.8	103
4	Electronic Structure and Spectroscopy of [Ru(tpy)₂]²⁺, [Ru(tpy)(bpy)(H₂O)]²⁺, and [Ru(tpy)(bpy)(Cl)]⁺. Inorganic Chemistry, 2009, 48, 10720-10725.	4.0	91
5	Interfacial Electron Transfer in TiO₂ Surfaces Sensitized with Ru(II)â^'Polypyridine Complexes. Journal of Physical Chemistry A, 2009, 113, 12532-12540.	2.5	80
6	Cyclometalated Fe(II) Complexes as Sensitizers in Dye-Sensitized Solar Cells. Inorganic Chemistry, 2015, 54, 560-569.	4.0	78
7	Fe(II)-Polypyridines as Chromophores in Dye-Sensitized Solar Cells: A Computational Perspective. Accounts of Chemical Research, 2015, 48, 1441-1449.	15.6	76
8	A flexible, redox-active macrocycle enables the electrocatalytic reduction of nitrate to ammonia by a cobalt complex. Chemical Science, 2018, 9, 4950-4958.	7.4	63
9	Density Functional Theory Study of Small Vanadium Oxide Clustersâ€. Journal of Physical Chemistry A, 2007, 111, 12938-12943.	2.5	62
10	Tuning the Electronic Structure of Fe(II) Polypyridines via Donor Atom and Ligand Scaffold Modifications: A Computational Study. Inorganic Chemistry, 2015, 54, 8786-8793.	4.0	61
11	Electron Injection from Copper Diimine Sensitizers into TiO₂: Structural Effects and Their Implications for Solar Energy Conversion Devices. Journal of the American Chemical Society, 2015, 137, 9670-9684.	13.7	60
12	HOMO inversion as a strategy for improving the light-absorption properties of Fe(<scp>ii</scp>) chromophores. Chemical Science, 2017, 8, 8115-8126.	7.4	52
13	Reactions of Sulfur Dioxide with Neutral Vanadium Oxide Clusters in the Gas Phase. II. Experimental Study Employing Single-Photon Ionization. Journal of Physical Chemistry A, 2008, 112, 11067-11077.	2.5	48
14	Elucidating Band-Selective Sensitization in Iron(II) Polypyridine-TiO₂ Assemblies. Inorganic Chemistry, 2013, 52, 8621-8628.	4.0	48
15	Insights into the Spin-State Transitions in [Fe(tpy)₂]²⁺: Importance of the Terpyridine Rocking Motion. Inorganic Chemistry, 2015, 54, 11259-11268.	4.0	47
16	Tuning the Redox Potentials and Ligand Field Strength of Fe(II) Polypyridines: The Dual Ï€-Donor and Ï€-Acceptor Character of Bipyridine. Inorganic Chemistry, 2018, 57, 9907-9917.	4.0	44
17	Intramolecular Hydrogen Bonding Facilitates Electrocatalytic Reduction of Nitrite in Aqueous Solutions. Inorganic Chemistry, 2019, 58, 9443-9451.	4.0	40
18	Reactions of Sulfur Dioxide with Neutral Vanadium Oxide Clusters in the Gas Phase. I. Density Functional Theory Study. Journal of Physical Chemistry A, 2007, 111, 13339-13346.	2.5	32

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19	Systematic Study of Modifications to Ruthenium(II) Polypyridine Dyads for Electron Injection Enhancement. Inorganic Chemistry, 2010, 49, 2975-2982.	4.0	31
20	Using Ultrafast X-ray Spectroscopy To Address Questions in Ligand-Field Theory: The Excited State Spin and Structure of [Fe(dcpp)₂]²⁺. Inorganic Chemistry, 2019, 58, 9341-9350.	4.0	29
21	Ray-Dutt and Bailar Twists in Fe(II)-Tris(2,2â€²-bipyridine): Spin States, Sterics, and Feâ€“N Bond Strengths. Inorganic Chemistry, 2018, 57, 5585-5596.	4.0	25
22	Exploration of Basis Set Issues for Calculation of Intermolecular Interactions. Journal of Physical Chemistry A, 2006, 110, 9529-9541.	2.5	20
23	Linker dependence of interfacial electron transfer rates in Fe(II)-polypyridine sensitized solar cells. Journal of Physics Condensed Matter, 2015, 27, 134205.	1.8	19
24	Electronic Structure and Absorption Properties of Strongly Coupled Porphyrinâ€“Perylene Arrays. Journal of Physical Chemistry A, 2015, 119, 9879-9888.	2.5	19
25	Influence of Electrolyte Composition on Ultrafast Interfacial Electron Transfer in Fe-Sensitized TiO₂-Based Solar Cells. Journal of Physical Chemistry C, 2020, 124, 1794-1811.	3.1	19
26	Two-step model for ultrafast interfacial electron transfer: limitations of Fermiâ€™s golden rule revealed by quantum dynamics simulations. Chemical Science, 2017, 8, 5979-5991.	7.4	17
27	Electrode-adsorption activates trans-[Cr(cyclam)Cl₂]⁺ for electrocatalytic nitrate reduction. Chemical Communications, 2020, 56, 603-606.	4.1	15
28	Role of a 3D Structure in Energy Transfer in Mixed-Ligand Metalâ€“Organic Frameworks. Journal of Physical Chemistry C, 2021, 125, 22998-23010.	3.1	15
29	Nondirected Câ€“H Activation of Arenes with Cp*Ir(III) Acetate Complexes: An Experimental and Computational Study. Organometallics, 2016, 35, 2435-2445.	2.3	13
30	Reaction Path Following with Sparse Interpolation. Journal of Chemical Theory and Computation, 2014, 10, 2942-2949.	5.3	12
31	Excited-State Switching between Ligand-Centered and Charge Transfer Modulated by Metalâ€“Carbon Bonds in Cyclopentadienyl Iridium Complexes. Inorganic Chemistry, 2018, 57, 15445-15461.	4.0	12
32	Designing air-stable cyclometalated Fe(<scp>ii</scp>) complexes: stabilization via electrostatic effects. Dalton Transactions, 2019, 48, 374-378.	3.3	12
33	Effects of Peripheral and Axial Substitutions on Electronic Transitions of Tin Naphthalocyanines. Journal of Physical Chemistry A, 2011, 115, 9265-9272.	2.5	11
34	Quantum Dynamics Simulations of Excited State Energy Transfer in a Zincâ€“Free-Base Porphyrin Dyad. Journal of Physical Chemistry A, 2016, 120, 8075-8084.	2.5	11
35	Interpolation Methods for Molecular Potential Energy Surface Construction. Journal of Physical Chemistry A, 2021, 125, 9725-9735.	2.5	11
36	Electronic Structure of Covalently Linked Zinc Bacteriochlorin Molecular Arrays: Insights into Molecular Design for NIR Light Harvesting. Journal of Physical Chemistry A, 2014, 118, 9901-9913.	2.5	10

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37	Orbital Analysis and Excited-State Calculations in an Energy-Based Fragmentation Method. Journal of Chemical Theory and Computation, 2013, 9, 3350-3363.	5.3	9
38	Comparison of Interfacial Electron Transfer Efficiency in [Fe(ctpy)₂]²⁺â€“TiO₂ and [Fe(cCNC)₂]²⁺â€“TiO₂ Assemblies: Importance of Conformational Sampling. Journal of Physical Chemistry A, 2018, 122, 1821-1830.	2.5	9
39	Evidence for a lowest energy ³MLCT excited state in [Fe(tpy)(CN)₃]^{â^'}. Chemical Communications, 2021, 57, 4658-4661.	4.1	9
40	Electrocatalytic nitrate reduction with Co-based catalysts: comparison of DIM, TIM and cyclam ligands. Dalton Transactions, 2021, 50, 12324-12331.	3.3	8
41	Role of Noncoplanar Conformation in Facilitating Ground State Hole Transfer in Oxidized Porphyrin Dyads. Journal of Physical Chemistry A, 2012, 116, 10107-10114.	2.5	6
42	Halogenation affects driving forces, reorganization energies and â€œrockingâ€•motions in strained [Fe(tpy)₂]²⁺ complexes. Dalton Transactions, 2021, 50, 14566-14575.	3.3	6
43	Molecular Dynamics Simulations on Relaxed Reduced-Dimensional Potential Energy Surfaces. Journal of Physical Chemistry A, 2019, 123, 4543-4554.	2.5	5
44	Ground-State Electronic Structure of RC-LH1 and LH2 Pigment Assemblies of Purple Bacteria via the EBF-MO Method. Journal of Physical Chemistry A, 2015, 119, 8934-8943.	2.5	4
45	Predicting the electrochemical behavior of Fe(II) complexes from ligand orbital energies. Journal of Photochemistry and Photobiology A: Chemistry, 2019, 376, 7-11.	3.9	4
46	Large Excited-State Conformational Displacements Expedite Triplet Formation in a Small Conjugated Oligomer. Journal of Physical Chemistry Letters, 2019, 10, 1259-1263.	4.6	4
47	The Influence of Nucleophilic and Redox Pincer Character as well as Alkali Metals on the Capture of Oxygen Substrates: The Case of Chromium(II). Chemistry - A European Journal, 2020, 26, 9547-9555.	3.3	4
48	The ligand-to-metal charge transfer excited state of [Re(dmpe)3]2+. Photosynthesis Research, 2022, 151, 155-161.	2.9	4
49	Electronic Absorption Spectra of Tetrapyrrole-Based Pigments via TD-DFT: A Reduced Orbital Space Study. Journal of Physical Chemistry A, 2016, 120, 5816-5825.	2.5	3
50	Approximating Periodic Potential Energy Surfaces with Sparse Trigonometric Interpolation. Journal of Physical Chemistry B, 2019, 123, 9677-9684.	2.6	3
51	SCC-DFTB Parameters for Feâ€“C Interactions. Journal of Physical Chemistry A, 2020, 124, 9674-9682.	2.5	3
52	Efficient Approximation of Potential Energy Surfaces with Mixed-Basis Interpolation. Journal of Chemical Theory and Computation, 2021, 17, 5673-5683.	5.3	3
53	Are all charge-transfer parameters created equally? A study of functional dependence and excited-state charge-transfer quantification across two dye families. Physical Chemistry Chemical Physics, 2021, 23, 20583-20597.	2.8	3
54	Electron transport through a (terpyridine)ruthenium metallo-surfactant containing a redox-active aminocatechol derivative. Dalton Transactions, 2022, 51, 8425-8436.	3.3	3

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55	Reduced-dimensional surface hopping with offlineâ€“online computations. Physical Chemistry Chemical Physics, 2021, 23, 19547-19557.	2.8	2
56	Investigating Interfacial Electron Transfer in Highly Efficient Porphyrin-Sensitized Solar Cells. ACS Symposium Series, 2015, , 169-188.	0.5	0