

# Lukas Bucinsky

## List of Publications by Year in descending order

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59  
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docs citations

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times ranked

1174  
citing authors

#	ARTICLE	IF	CITATIONS
1	Quantum Crystallography: Current Developments and Future Perspectives. Chemistry - A European Journal, 2018, 24, 10881-10905.	3.3	108
2	Importance of Relativistic Effects and Electron Correlation in Structure Factors and Electron Density of Diphenyl Mercury and Triphenyl Bismuth. Journal of Physical Chemistry A, 2016, 120, 6650-6669.	2.5	57
3	X-ray constrained unrestricted Hartree-Fock and Douglas-Kroll-Hess wavefunctions. Acta Crystallographica Section A: Foundations and Advances, 2010, 66, 78-92.	0.3	44
4	Spectroscopic and Computational Studies of Spin States of Iron(IV) Nitrido and Imido Complexes. Inorganic Chemistry, 2017, 56, 4751-4768.	4.0	41
5	NO Releasing and Anticancer Properties of Octahedral Ruthenium-Nitrosyl Complexes with Equatorial 1 <i>H</i> -Indazole Ligands. Inorganic Chemistry, 2018, 57, 10702-10717.	4.0	34
6	Copper(II) complexes with new fluoroquinolones: Synthesis, structure, spectroscopic and theoretical study, DNA damage, cytotoxicity and antiviral activity. Journal of Inorganic Biochemistry, 2015, 150, 160-173.	3.5	30
7	Redox Reactions of Nickel, Copper, and Cobalt Complexes with "Noninnocent" Dithiolate Ligands: Combined in Situ Spectroelectrochemical and Theoretical Study. Organometallics, 2014, 33, 4846-4859.	2.3	29
8	Charge and Spin States in Schiff Base Metal Complexes with a Disiloxane Unit Exhibiting a Strong Noninnocent Ligand Character: Synthesis, Structure, Spectroelectrochemistry, and Theoretical Calculations. Inorganic Chemistry, 2015, 54, 5691-5706.	4.0	29
9	Relativistic Effects on Metal-Metal Bonding: Comparison of the Performance of ECP and Scalar DKH Description on the Picture of Metal-Metal Bonding in $\text{Re}_2\text{Cl}_8^{2+}$ . Journal of Chemical Theory and Computation, 2010, 6, 3113-3121.	5.3	28
10	Conformational, Spectroscopic, and Molecular Dynamics DFT Study of Precursors for New Potential Antibacterial Fluoroquinolone Drugs. Journal of Physical Chemistry A, 2014, 118, 9540-9551.	2.5	26
11	On relativistic effects in ground state potential curves of $\text{Zn}_2$ , $\text{Cd}_2$ , and $\text{Hg}_2$ dimers. A CCSD(T) study. Journal of Computational Chemistry, 2009, 30, 65-74.	3.3	24
12	Relativistic quantum crystallography of diphenyl- and dicyanomercuro. Theoretical structure factors and Hirshfeld atom refinement. Acta Crystallographica Section A: Foundations and Advances, 2019, 75, 705-717.	0.1	23
13	Ligand Substituent Effects in Manganese Pyridinophane Complexes: Implications for Oxygen-Evolving Catalysis. Inorganic Chemistry, 2017, 56, 14315-14325.	4.0	22
14	A five-coordinate manganese(III) complex of a salen type ligand with a positive axial anisotropy parameter D. Dalton Transactions, 2017, 46, 11817-11829.	3.3	20
15	On the Electronic Structure of <i>mer</i> , <i>trans</i> - $[\text{RuCl}_3(\text{1H-indazole})_2(\text{NO})]$ , a Hypothetical Metabolite of the Antitumor Drug Candidate KP1019: An Experimental and DFT Study. European Journal of Inorganic Chemistry, 2013, 2013, 2505-2519.	2.0	18
16	Nickel(II) Complexes with Redox Noninnocent Octaazamacrocycles as Catalysts in Oxidation Reactions. Inorganic Chemistry, 2019, 58, 11133-11145.	4.0	16
17	Impact of Substituent Variation on the Presence of Thermal Spin Crossover in a Series of Mononuclear Iron(III) Schiff Base Complexes with Terminal Pseudohalido Co-ligands. Chemistry - A European Journal, 2018, 24, 5191-5203.	3.3	15
18	3CLpro and PLpro affinity, a docking study to fight COVID19 based on 900 compounds from PubChem and literature. Are there new drugs to be found?. Journal of Molecular Structure, 2021, 1245, 130968.	3.6	15

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19	On the origin of the hemidirected geometry of tetracoordinated lead(II) compounds. <i>Chemical Physics</i> , 2010, 368, 14-19.	1.9	14
20	Picture change error correction of radon atom electron density. <i>Journal of Chemical Physics</i> , 2010, 133, 174125.	3.0	14
21	Study of the picture change error at the 2nd order Douglas Kroll Hess level of theory. Electron and spin density and structure factors of the Bis[bis(methoxycarbimido) aminato] copper (II) complex. <i>Chemical Physics</i> , 2012, 395, 44-53.	1.9	14
22	Picture change error in quasirelativistic electron/spin density, Laplacian and bond critical points. <i>Chemical Physics</i> , 2014, 438, 37-47.	1.9	14
23	Electronic structure of two isostructural 'paddle-wheel' complexes: a comparative study. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2018, 74, 681-692.	1.1	14
24	Picture change error correction in the radial distributions of canonical orbital densities and total electron density of radon atom: the effect of the size of nucleus and the basis set limit. <i>Theoretical Chemistry Accounts</i> , 2011, 129, 181-197.	1.4	11
25	HFEPR and Computational Studies on the Electronic Structure of a High-Spin Oxidiron(IV) Complex in Solution. <i>Inorganic Chemistry</i> , 2016, 55, 3933-3945.	4.0	11
26	cis-Tetrachlorido-bis(indazole)osmium(IV) and its osmium(III) analogues: paving the way towards the cis-isomer of the ruthenium anticancer drugs KP1019 and/or NKP1339. <i>Dalton Transactions</i> , 2017, 46, 11925-11941.	3.3	11
27	High-Frequency and -Field EPR (HFEPR) Investigation of a Pseudotetrahedral Cr <sup>IV</sup> Siloxide Complex and Computational Studies of Related Cr <sup>IV</sup> L <sub>4</sub> Systems. <i>Inorganic Chemistry</i> , 2019, 58, 4907-4920.	4.0	11
28	Spin contamination analogy, Kramers pairs symmetry and spin density representations at the 2-component unrestricted Hartree-Fock level of theory. <i>Computational and Theoretical Chemistry</i> , 2015, 1065, 27-41.	2.5	10
29	Detection of simple inorganic and organic molecules over Cu-decorated circumcoronene: a combined DFT and QTAIM study. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 16021-16032.	2.8	10
30	Dinuclear manganese(III) complexes with bioinspired coordination and variable linkers showing weak exchange effects: a synthetic, structural, spectroscopic and computation study. <i>Dalton Transactions</i> , 2019, 48, 5909-5922.	3.3	10
31	On the hydrogen storage performance of Cu-doped and Cu-decorated graphene quantum dots: a computational study. <i>Theoretical Chemistry Accounts</i> , 2020, 139, 1.	1.4	10
32	Machine learning prediction of 3CL SARS-CoV-2 docking scores. <i>Computational Biology and Chemistry</i> , 2022, 98, 107656.	2.3	9
33	Relativistic effects in HgHe and HgXe CCSD(T) ground state potential curves. Low-density viscosity simulations of Hg:Xe mixture. <i>Journal of Computational Chemistry</i> , 2011, 32, 356-367.	3.3	8
34	Redox processes of 2,6-dichlorophenolindophenolate in different solvents. A combined electrochemical, spectroelectrochemical, photochemical, and theoretical study. <i>Journal of Solid State Electrochemistry</i> , 2015, 19, 2633-2642.	2.5	8
35	Theoretical study of hydrogen adsorption on the graphene quantum dots doped with various first row transition metals: Switch of spin state as a way to improve H <sub>2</sub> adsorption. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2022, 139, 115144.	2.7	8
36	Coordination bonding in dicopper and dichromium tetrakis(1/4 acetato) aqua complexes: Nature, strength, length, and topology. <i>Journal of Computational Chemistry</i> , 2020, 41, 698-714.	3.3	7

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37	The Ruthenium Nitrosyl Moiety in Clusters: Trinuclear Linear $\mu_3$ -Hydroxo Magnesium(II)-Diruthenium(II), $\mu_3$ -Oxido Trinuclear Diiron(III) $\mu_3$ -Ruthenium(II), and Tetranuclear $\mu_4$ -Oxido Trigallium(III)-Ruthenium(II) Complexes. <i>Inorganic Chemistry</i> , 2022, 61, 950-967.	4.0	7
38	New quantum number for the many-electron Dirac-Coulomb Hamiltonian. <i>Physical Review A</i> , 2016, 94, .	2.5	6
39	Molecular docking and machine learning affinity prediction of compounds identified upon softwood bark extraction to the main protease of the SARS-CoV-2 virus. <i>Biophysical Chemistry</i> , 2022, 288, 106854.	2.8	6
40	Spectroelectrochemical, photochemical and theoretical study of octaazamacrocyclic nickel(II) complexes exhibiting unusual solvent-dependent deprotonation of methylene group. <i>Electrochimica Acta</i> , 2019, 326, 135006.	5.2	5
41	Diastereomeric dinickel( $\mu_2$ ) complexes with non-innocent bis(octaazamacrocyclic) ligands: isomerization, spectroelectrochemistry, DFT calculations and use in catalytic oxidation of cyclohexane. <i>Dalton Transactions</i> , 2022, 51, 5151-5167.	3.3	5
42	The quasirelativistic contact interaction and effective electron and spin densities at the nucleus: A model based on weighting the electron density with the finite Gaussian nucleus model. <i>Chemical Physics Letters</i> , 2013, 580, 152-159.	2.6	4
43	Calculations of hyperfine coupling constant of copper(II) in aqueous environment. Finite temperature molecular dynamics and relativistic effects. <i>Journal of Molecular Modeling</i> , 2015, 21, 237.	1.8	4
44	Joined X-ray, spectroscopic and theoretical study of potential antibacterial cyano group containing fluoroquinolone drugs precursors with the focus on the conformational behavior. <i>Journal of Molecular Structure</i> , 2016, 1125, 736-750.	3.6	4
45	Hg $\mu_2$ meets relativistic quantum crystallography. How to teach relativity to a non-relativistic wavefunction. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2021, 77, 54-66.	0.1	4
46	Cathodic and Photocatalytic Reduction of Nitroquinolones Investigated by In Situ EPR/UV-Vis Spectroelectrochemistry and EPR spectroscopy. <i>Current Organic Chemistry</i> , 2013, 17, 2427-2439.	1.6	4
47	Additivity in kramers pairs symmetry: Multiplets with up to four unpaired electrons. <i>International Journal of Quantum Chemistry</i> , 2016, 116, 1040-1048.	2.0	3
48	Protonation and electronic structure of 2,6-dichlorophenolindophenolate during reduction. A theoretical study including explicit solvent. <i>Journal of Molecular Modeling</i> , 2016, 22, 251.	1.8	3
49	Structure functionality relationship of flavonoids (myricetin, morin, taxifolin and) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 267 T Structure, 2020, 1222, 128923.	3.6	3
50	Charge density of 4-methyl-3-[(tetrahydro-2 <i>H</i> -pyran-2-yl)oxy]thiazole-2(3 <i>H</i> )-thione. A comprehensive multipole refinement, maximum entropy method and density functional theory study. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2020, 76, 450-468.	1.1	3
51	Ni Oxidation State and Ligand Saturation Impact on the Capability of Octaazamacrocyclic Complexes to Bind and Reduce CO <sub>2</sub> . <i>Molecules</i> , 2021, 26, 4139.	3.8	3
52	On the diffusion coefficients and stability of van der Waals complex Hg $\mu_2$ . <i>International Journal of Quantum Chemistry</i> , 2008, 108, 2150-2158.	2.0	2
53	Electronic structure of Schiff-base peroxo{2,2- $\eta^2$ -[1,2-phenylenebis(nitrilomethanylylidene)]bis(6-methoxyphenolato)}titanium(IV) monohydrate: a possible model structure of the reaction center for the theoretical study of hemoglobin. <i>IUCr</i> , 2021, 8, 295-304.	2.2	2
54	Ab initio X10+ground state potential curves of Pb $\mu_2$ dimers (RG = He, Ne, Ar) including spin-orbit effects. Simulation of diffusion coefficients. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 18519.	2.8	1

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55	Frontispiece: Quantum Crystallography: Current Developments and Future Perspectives. Chemistry - A European Journal, 2018, 24, .	3.3	1
56	Copper atom representation in charge density analysis of (5-chlorosalicylate)-(2,9-dimethylphenanthroline)-(aqua) copper complex: Experimental and theoretical study. Journal of Molecular Structure, 2017, 1135, 186-196.	3.6	0
57	General build up of basis and matrix in the diagonalization approach. Determination of Kramers configuration state functions. International Journal of Quantum Chemistry, 2018, 118, e25638.	2.0	0
58	Finite nucleus effects, relativistic effects and picture change error in the IOTC/DKH2 contact spin densities of Cu, Ag, Au atoms. Acta Chimica Slovaca, 2014, 7, 65-72.	0.8	0