Lukas Bucinsky

List of Publications by Year
in descending order

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58	843	567281	552781
papers	citations	15 h-index	26 g-index

59	59	59	1174
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	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 H2 adsorption. Physica E: Low-Dimensional Systems and Nanostructures, 2022, 139, 115144.	2.7	8
2	Diastereomeric dinickel(<scp>ii</scp>) complexes with non-innocent bis(octaazamacrocyclic) ligands: isomerization, spectroelectrochemistry, DFT calculations and use in catalytic oxidation of cyclohexane. Dalton Transactions, 2022, 51, 5151-5167.	3.3	5
3	Machine learning prediction of 3CL SARS-CoV-2 docking scores. Computational Biology and Chemistry, 2022, 98, 107656.	2.3	9
4	The Ruthenium Nitrosyl Moiety in Clusters: Trinuclear Linear Î¼-Hydroxido Magnesium(II)-Diruthenium(II), Î¼₃-Oxido Trinuclear Diiron(III)â€“Ruthenium(II), and Tetranuclear Î¼₄-Oxido Trigallium(III)-Ruthenium(II) Complexes. Inorganic Chemistry, 2022, 61, 950-967.	4.0	7
5	Molecular docking and machine learning affinity prediction of compounds identified upon softwood bark extraction to the main protease of the SARS-CoV-2 virus. Biophysical Chemistry, 2022, 288, 106854.	2.8	6
6	HgH₂meets relativistic quantum crystallography. How to teach relativity to a non-relativistic wavefunction. Acta Crystallographica Section A: Foundations and Advances, 2021, 77, 54-66.	0.1	4
7	Electronic structure of Schiff-base peroxo{2,2â€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. IUCrJ, 2021, 8, 295-304.	2.2	2
8	Ni Oxidation State and Ligand Saturation Impact on the Capability of Octaazamacrocyclic Complexes to Bind and Reduce CO2. Molecules, 2021, 26, 4139.	3.8	3
9	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
10	Coordination bonding in dicopper and dichromium tetrakis(Î¼â€acetato)â€diaqua complexes: Nature, strength, length, and topology. Journal of Computational Chemistry, 2020, 41, 698-714.	3.3	7
11	On the hydrogen storage performance of Cu-doped and Cu-decorated graphene quantum dots: a computational study. Theoretical Chemistry Accounts, 2020, 139, 1.	1.4	10
12	Structure functionality relationship of flavonoids (myricetin, morin, taxifolin and) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 307 Td (3â€²,4â€ Structure, 2020, 1222, 128923.	3.6	3
13	Charge density of 4-methyl-3-[(tetrahydro-2H-pyran-2-yl)oxy]thiazole-2(3H)-thione. A comprehensive multipole refinement, maximum entropy method and density functional theory study. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2020, 76, 450-468.	1.1	3
14	Nickel(II) Complexes with Redox Noninnocent Octaazamacrocycles as Catalysts in Oxidation Reactions. Inorganic Chemistry, 2019, 58, 11133-11145.	4.0	16
15	Spectroelectrochemical, photochemical and theoretical study of octaazamacrocyclic nickel(II) complexes exhibiting unusual solvent-dependent deprotonation of methylene group. Electrochimica Acta, 2019, 326, 135006.	5.2	5
16	Relativistic quantum crystallography of diphenyl- and dicyanomercury. Theoretical structure factors and Hirshfeld atom refinement. Acta Crystallographica Section A: Foundations and Advances, 2019, 75, 705-717.	0.1	23
17	Dinuclear manganese(iii) complexes with bioinspired coordination and variable linkers showing weak exchange effects: a synthetic, structural, spectroscopic and computation study. Dalton Transactions, 2019, 48, 5909-5922.	3.3	10
18	High-Frequency and -Field EPR (HFEPR) Investigation of a Pseudotetrahedral Cr^{IV} Siloxide Complex and Computational Studies of Related Cr^{IV}L₄ Systems. Inorganic Chemistry, 2019, 58, 4907-4920.	4.0	11

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19	Quantum Crystallography: Current Developments and Future Perspectives. Chemistry - A European Journal, 2018, 24, 10881-10905.	3.3	108
20	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
21	Impact of Substituent Variation on the Presence of Thermal Spin Crossover in a Series of Mononuclear Iron(III) Schiff Base Complexes with Terminal Pseudohalido Coâ€ligands. Chemistry - A European Journal, 2018, 24, 5191-5203.	3.3	15
22	Detection of simple inorganic and organic molecules over Cu-decorated circumcoronene: a combined DFT and QTAIM study. Physical Chemistry Chemical Physics, 2018, 20, 16021-16032.	2.8	10
23	Frontispiece: Quantum Crystallography: Current Developments and Future Perspectives. Chemistry - A European Journal, 2018, 24, .	3.3	1
24	NO Releasing and Anticancer Properties of Octahedral Rutheniumâ€“Nitrosyl Complexes with Equatorial 1H-Indazole Ligands. Inorganic Chemistry, 2018, 57, 10702-10717.	4.0	34
25	Electronic structure of two isostructural `paddle-wheel' complexes: a comparative study. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2018, 74, 681-692.	1.1	14
26	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
27	Spectroscopic and Computational Studies of Spin States of Iron(IV) Nitrido and Imido Complexes. Inorganic Chemistry, 2017, 56, 4751-4768.	4.0	41
28	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. Dalton Transactions, 2017, 46, 11925-11941.	3.3	11
29	A five-coordinate manganese(<scp>iii</scp>) complex of a salen type ligand with a positive axial anisotropy parameter D. Dalton Transactions, 2017, 46, 11817-11829.	3.3	20
30	Ligand Substituent Effects in Manganese Pyridinophane Complexes: Implications for Oxygen-Evolving Catalysis. Inorganic Chemistry, 2017, 56, 14315-14325.	4.0	22
31	Additivity in kramers pairs symmetry: Multiplets with up to four unpaired electrons. International Journal of Quantum Chemistry, 2016, 116, 1040-1048.	2.0	3
32	New quantum number for the many-electron Dirac-Coulomb Hamiltonian. Physical Review A, 2016, 94, .	2.5	6
33	HFEPR and Computational Studies on the Electronic Structure of a High-Spin Oxidoiron(IV) Complex in Solution. Inorganic Chemistry, 2016, 55, 3933-3945.	4.0	11
34	Protonation and electronic structure of 2,6-dichlorophenolindophenolate during reduction. A theoretical study including explicit solvent. Journal of Molecular Modeling, 2016, 22, 251.	1.8	3
35	Joined X-ray, spectroscopic and theoretical study of potential antibacterial cyano group containing fluoroquinolone drugs precursors with the focus on the conformational behavior. Journal of Molecular Structure, 2016, 1125, 736-750.	3.6	4
36	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

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37	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
38	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
39	Spin contamination analogy, Kramers pairs symmetry and spin density representations at the 2-component unrestricted Hartreeâ€“Fock level of theory. Computational and Theoretical Chemistry, 2015, 1065, 27-41.	2.5	10
40	Redox processes of 2,6-dichlorophenolindophenolate in different solvents. A combined electrochemical, spectroelectrochemical, photochemical, and theoretical study. Journal of Solid State Electrochemistry, 2015, 19, 2633-2642.	2.5	8
41	Calculations of hyperfine coupling constant of copper(II) in aqueous environment. Finite temperature molecular dynamics and relativistic effects. Journal of Molecular Modeling, 2015, 21, 237.	1.8	4
42	Ab initio X10+ground state potential curves of Pbâ¯RG dimers (RG = He, Ne, Ar) including spinâ€“orbit effects. Simulation of diffusion coefficients. Physical Chemistry Chemical Physics, 2014, 16, 18519.	2.8	1
43	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
44	Redox Reactions of Nickel, Copper, and Cobalt Complexes with â€œNoninnocentâ€•Dithiolate Ligands: Combined in Situ Spectroelectrochemical and Theoretical Study. Organometallics, 2014, 33, 4846-4859.	2.3	29
45	Picture change error in quasirelativistic electron/spin density, Laplacian and bond critical points. Chemical Physics, 2014, 438, 37-47.	1.9	14
46	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
47	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. Chemical Physics Letters, 2013, 580, 152-159.	2.6	4
48	On the Electronic Structure of mer,transâ€[RuCl₃(1Hâ€indazole)₂(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
49	Cathodic and Photocatalytic Reduction of Nitroquinolones Investigated by In Situ EPR/UV-Vis Spectroelectrochemistry and EPR spectroscopy. Current Organic Chemistry, 2013, 17, 2427-2439.	1.6	4
50	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. Chemical Physics, 2012, 395, 44-53.	1.9	14
51	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. Theoretical Chemistry Accounts, 2011, 129, 181-197.	1.4	11
52	Relativistic effects in HgHe and HgXe CCSD(T) ground state potential curves. Lowâ€density viscosity simulations of Hg:Xe mixture. Journal of Computational Chemistry, 2011, 32, 356-367.	3.3	8
53	On the origin of the hemidirected geometry of tetracoordinated lead(II) compounds. Chemical Physics, 2010, 368, 14-19.	1.9	14
54	X-ray constrained unrestricted Hartreeâ€“Fock and Douglasâ€“Krollâ€“Hess wavefunctions. Acta Crystallographica Section A: Foundations and Advances, 2010, 66, 78-92.	0.3	44

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55	Picture change error correction of radon atom electron density. Journal of Chemical Physics, 2010, 133, 174125.	3.0	14
56	Relativistic Effects on Metalâ^'Metal Bonding: Comparison of the Performance of ECP and Scalar DKH Description on the Picture of Metalâ^'Metal Bonding in Re₂Cl₈^{2â^'}. Journal of Chemical Theory and Computation, 2010, 6, 3113-3121.	5.3	28
57	On relativistic effects in ground state potential curves of Zn₂, Cd₂, and Hg₂ dimers. A CCSD(T) study. Journal of Computational Chemistry, 2009, 30, 65-74.	3.3	24
58	On the diffusion coefficients and stability of van der Waals complex Hgâ€¦ N₂. International Journal of Quantum Chemistry, 2008, 108, 2150-2158.	2.0	2