Jakub Sebera

List of Publications by Year
in descending order

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56	1,399	394390	330122
papers	citations	19	37
		h-index	g-index

59	59	59	1890
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	The <scp>Adâ€MD</scp> method to calculate <scp>NMR</scp> shift including effects due to conformational dynamics: The <scp>³¹P NMR</scp> shift in <scp>DNA</scp>. Journal of Computational Chemistry, 2022, 43, 132-143.	3.3	5
2	Quantitative Analysis of Nanorough Hydrogenated Si(111) Surfaces through Vibrational Spectral Assignment by Periodic DFT Calculations. Journal of Physical Chemistry C, 2022, 126, 8278-8286.	3.1	0
3	Environmental Control of Singleâ€Molecule Junction Evolution and Conductance: A Case Study of Expanded Pyridinium Wiring. Angewandte Chemie - International Edition, 2021, 60, 4732-4739.	13.8	8
4	Environmental Control of Singleâ€Molecule Junction Evolution and Conductance: A Case Study of Expanded Pyridinium Wiring. Angewandte Chemie, 2021, 133, 4782-4789.	2.0	2
5	Does the Seebeck coefficient of a single-molecule junction depend on the junction configuration?. Journal of Materials Chemistry A, 2021, 9, 17512-17520.	10.3	4
6	FTIR Measurement of the Hydrogenated Si(100) Surface: The Structure-Vibrational Interpretation by Means of Periodic DFT Calculation. Journal of Physical Chemistry C, 2021, 125, 9219-9228.	3.1	2
7	Raman spectroscopy and DFT calculations of PEDOT:PSS in a dipolar field. Physical Chemistry Chemical Physics, 2021, 24, 541-550.	2.8	24
8	HERMES â€“ A Software Tool for the Prediction and Analysis of Magneticâ€Fieldâ€Induced Residual Dipolar Couplings in Nucleic Acids. ChemPlusChem, 2020, 85, 2177-2185.	2.8	0
9	Interstrand Charge Transport within Metallo-DNA: the Effect Due to Hg(II)- and Ag(I)-Mediated Base Pairs. Journal of Physical Chemistry C, 2020, 124, 7477-7486.	3.1	2
10	QM and QM/MM umbrella sampling MD study of the formation of Hg(II)â€“thymine bond: Model for evaluation of the reaction energy profiles in solutions with constant pH. Journal of Computational Chemistry, 2020, 41, 1509-1520.	3.3	1
11	Electrochemical characterization of the artificial metalloenzyme papain-[(Î·6-arene)Ru(1,10-phenanthroline)Cl]+. Journal of Electroanalytical Chemistry, 2020, 859, 113882.	3.8	1
12	Investigation of the charge transport in model single molecule junctions based on expanded bipyridinium molecular conductors. Electrochimica Acta, 2019, 301, 267-273.	5.2	11
13	Tuning the contact conductance of anchoring groups in single molecule junctions by molecular design. Nanoscale, 2019, 11, 12959-12964.	5.6	6
14	Structural interpretation of the ³¹P NMR chemical shifts in thiophosphate and phosphate: key effects due to spinâ€“orbit and explicit solvent. Physical Chemistry Chemical Physics, 2019, 21, 9924-9934.	2.8	11
15	Probabilistic mapping of single molecule junction configurations as a tool to achieve the desired geometry of asymmetric tripodal molecules. Chemical Communications, 2019, 55, 3351-3354.	4.1	12
16	Single Molecule Conductance of Electroactive Helquats: Solvent Effect. ChemElectroChem, 2019, 6, 5856-5863.	3.4	5
17	Correlation of electrochemical properties of expanded pyridinium compounds with their single molecule conductance. Electrochimica Acta, 2018, 264, 301-311.	5.2	12
18	The structural model of Zika virus RNA-dependent RNA polymerase in complex with RNA for rational design of novel nucleotide inhibitors. Scientific Reports, 2018, 8, 11132.	3.3	26

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19	The mechanism of the glycosylase reaction with hOGG1 base-excision repair enzyme: concerted effect of Lys249 and Asp268 during excision of 8-oxoguanine. Nucleic Acids Research, 2017, 45, 5231-5242.	14.5	19
20	Tuning Charge Transport Properties of Asymmetric Molecular Junctions. Journal of Physical Chemistry C, 2017, 121, 12885-12894.	3.1	36
21	Theoretical and experimental study of the antifreeze protein AFP752, trehalose and dimethyl sulfoxide cryoprotection mechanism: correlation with cryopreserved cell viability. RSC Advances, 2017, 7, 352-360.	3.6	50
22	Investigation of the geometrical arrangement and single molecule charge transport in self-assembled monolayers of molecular towers based on tetraphenylmethane tripod. Electrochimica Acta, 2017, 258, 1191-1200.	5.2	17
23	The benchmark of ³¹P NMR parameters in phosphate: a case study on structurally constrained and flexible phosphate. Physical Chemistry Chemical Physics, 2017, 19, 31830-31841.	2.8	17
24	The growth of zinc phthalocyanine thin films by pulsed laser deposition. Journal of Materials Research, 2016, 31, 163-172.	2.6	19
25	Structure Determination of an Ag^Iâ€Mediated Cytosineâ€“Cytosine Base Pair within DNA Duplex in Solution with ¹H/¹⁵N/¹⁰⁹Ag NMR Spectroscopy. Chemistry - A European Journal, 2016, 22, 13028-13031.	3.3	63
26	The effect of chemical modification of DNA base on binding of HgII and AgI in metal-mediated base pairs. Inorganica Chimica Acta, 2016, 452, 199-204.	2.4	2
27	HgII/AgI-mediated base pairs and their NMR spectroscopic studies. Inorganica Chimica Acta, 2016, 452, 34-42.	2.4	19
28	Impact of nucleic acid self-alignment in a strong magnetic field on the interpretation of indirect spinâ€“spin interactions. Journal of Biomolecular NMR, 2016, 64, 53-62.	2.8	6
29	Benchmark Theoretical and Experimental Study on ¹⁵N NMR Shifts of Oxidatively Damaged Guanine. Journal of Physical Chemistry B, 2016, 120, 915-925.	2.6	10
30	Direct detection of the mercuryâ€“nitrogen bond in the thymineâ€“Hg^{II}â€“thymine base-pair with ¹⁹⁹Hg NMR spectroscopy. Chemical Communications, 2015, 51, 8488-8491.	4.1	36
31	Structures, physicochemical properties, and applications of Tâ€“Hg^{II}â€“T, Câ€“Ag^Iâ€“C, and other metallo-base-pairs. Chemical Communications, 2015, 51, 17343-17360.	4.1	136
32	The structure of metallo-DNA with consecutive thymineâ€“HgIIâ€“thymine base pairs explains positive entropy for the metallo base pair formation. Nucleic Acids Research, 2014, 42, 4094-4099.	14.5	106
33	The activation of N-glycosidic bond cleavage performed by base-excision repair enzyme hOGG1; theoretical study of the role of Lys 249 residue in activation of G, OxoG and FapyG. RSC Advances, 2014, 4, 44043-44051.	3.6	6
34	Magnetical and Optical Properties of Nanodiamonds Can Be Tuned by Particles Surface Chemistry: Theoretical and Experimental Study. Journal of Physical Chemistry C, 2014, 118, 25245-25252.	3.1	25
35	Theoretical and Experimental Study of Charge Transfer through DNA: Impact of Mercury Mediated T-Hg-T Base Pair. Journal of Physical Chemistry B, 2014, 118, 5374-5381.	2.6	41
36	Conductivity of boron-doped polycrystalline diamond films: influence of specific boron defects. European Physical Journal B, 2013, 86, 1.	1.5	55

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37	Formation of a Thymineâ€Hg^{II}â€Thymine Metalâ€Mediated DNA Base Pair: Proposal and Theoretical Calculation of the Reaction Pathway. Chemistry - A European Journal, 2013, 19, 9884-9894.	3.3	45
38	Charge transfer through DNA/DNA duplexes and DNA/RNA hybrids: Complex theoretical and experimental studies. Biophysical Chemistry, 2013, 180-181, 127-134.	2.8	11
39	Interaction of selected gases with zinc phthalocyanine thin films: theoretical and experimental studies. EPJ Applied Physics, 2013, 64, 10202.	0.7	8
40	Pyramidalization of the Glycosidic Nitrogen Provides the Way for Efficient Cleavage of the N-Glycosidic Bond of 8-OxoG with the hOGG1 DNA Repair Protein. Journal of Physical Chemistry B, 2012, 116, 12535-12544.	2.6	13
41	Polaron binding energy in polymers: poly[methyl(phenyl)silylene]. Journal of Molecular Modeling, 2012, 18, 623-629.	1.8	7
42	Charge transfer in porphyrinâ€“calixarene complexes: ultrafast kinetics, cyclic voltammetry, and DFT calculations. Physical Chemistry Chemical Physics, 2011, 13, 6947.	2.8	19
43	Charge carrier mobility in poly[methyl(phenyl)silylene] studied by time-resolved terahertz spectroscopy and molecular modelling. Physical Chemistry Chemical Physics, 2011, 13, 2850-2856.	2.8	13
44	Fine tuning of the catalytic effect of a metal-free porphyrin on the homogeneous oxygenreduction. Chemical Communications, 2011, 47, 5446-5448.	4.1	31
45	Polaron dynamics in molecular polysilane wires. Materials Research Innovations, 2011, 15, s232-s235.	2.3	0
46	Charge-transfer in some physical processes. Journal of Physics: Conference Series, 2010, 253, 012005.	0.4	0
47	Electrochemical and density functional studies of the catalytic ethylene oxidation on nanostructured Au electrodes. Catalysis Today, 2010, 158, 29-34.	4.4	18
48	The fluorescence of variously terminated nanodiamond particles: Quantum chemical calculations. Physica Status Solidi (A) Applications and Materials Science, 2010, 207, 2045-2048.	1.8	11
49	Charge Transport in DNA Oligonucleotides with Various Base-Pairing Patterns. Journal of Physical Chemistry B, 2010, 114, 5196-5205.	2.6	34
50	Fluorescent Nanodiamonds: Effect of Surface Termination. Materials Research Society Symposia Proceedings, 2009, 1203, 1.	0.1	2
51	Charge carrier mobility in sulphonated and non-sulphonated Ni phthalocyanines: experiment and quantum chemical calculations. European Physical Journal B, 2009, 72, 385-395.	1.5	23
52	How do vibrations change their composition upon electronic excitation? â€“ EXSY-T2D-IR measurements challenge DFT calculations.. Springer Series in Chemical Physics, 2009, , 421-423.	0.2	0
53	New organic FET-like photoactive device, experiments and DFT modeling. European Physical Journal E, 2008, 25, 299-307.	1.6	21
54	Femtosecond Fluorescence and Intersystem Crossing in Rhenium(I) Carbonylâ^'Bipyridine Complexes. Journal of the American Chemical Society, 2008, 130, 8967-8974.	13.7	269

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55	Ligand-to-Diimine/Metal-to-Diimine Charge-Transfer Excited States of [Re(NCS)(CO)3(Î±-diimine)] (Î±-diimine) Tj ETQq1 1 0.784314 rgBT Physical Chemistry A, 2005, 109, 5016-5025.	2.5	68
56	New rotationâ€“vibration band and potential energy function of NeH+ in the ground electronic state. Journal of Molecular Structure, 2004, 695-696, 5-11.	3.6	11