KÄstutis Aidas

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/7831601/publications.pdf

Version: 2024-02-01

48 papers	2,670 citations	448610 19 h-index	232693 48 g-index
48 all docs	48 docs citations	48 times ranked	3261 citing authors

#	Article	IF	Citations
1	Solid-State NMR and Impedance Spectroscopy Study of Spin Dynamics in Proton-Conducting Polymers: An Application of Anisotropic Relaxing Model. Journal of Physical Chemistry B, 2021, 125, 12592-12602.	1.2	5
2	Structural Features of the [C4mim][Cl] Ionic Liquid and Its Mixtures with Water: Insight from a 1H NMR Experimental and QM/MD Study. Journal of Physical Chemistry B, 2021, 125, 13255-13266.	1.2	7
3	CP MAS kinetics in soft matter: Spin diffusion, local disorder and thermal equilibration in poly(2-hydroxyethyl methacrylate). Solid State Nuclear Magnetic Resonance, 2020, 105, 101641.	1.5	10
4	Magnetic excitation and readout of methyl group tunnel coherence. Science Advances, 2020, 6, eaba1517.	4.7	16
5	Prediction of the tautomer stability and acidity of phenacylpyridines in aqueous solution. Theoretical Chemistry Accounts, 2020, 139, 1.	0.5	1
6	Computational NMR Study of Ion Pairing of 1-Decyl-3-methyl-imidazolium Chloride in Molecular Solvents. Journal of Physical Chemistry B, 2020, 124, 10776-10786.	1.2	6
7	Molecular aggregation in liquid acetic acid: insight from molecular dynamics/quantum mechanics modelling of structural and NMR properties. Physical Chemistry Chemical Physics, 2019, 21, 14811-14820.	1.3	12
8	NMR, Raman, and DFT Study of Lyotropic Chromonic Liquid Crystals of Biomedical Interest: Tautomeric Equilibrium and Slow Self-Assembling in Sunset Yellow Aqueous Solutions. Journal of Physical Chemistry B, 2018, 122, 3047-3055.	1.2	11
9	Electron paramagnetic resonance of a copper doped [(CH₃)₂NH₂][Zn(HCOO)₃] hybrid perovskite framework. Physical Chemistry Chemical Physics, 2018, 20, 12097-12105.	1.3	14
10	Pulse EPR and ENDOR Study of Manganese Doped [(CH₃)₂NH₂][Zn(HCOO)₃] Hybrid Perovskite Framework. Journal of Physical Chemistry C, 2017, 121, 27225-27232.	1.5	20
11	Aqueous acidities of primary benzenesulfonamides: Quantum chemical predictions based on density functional theory and SMD. Journal of Computational Chemistry, 2015, 36, 2158-2167.	1.5	10
12	FTIR/PCA study of propanol in argon matrix: The initial stage of clustering and conformational transitions. Low Temperature Physics, 2014, 40, 1077-1082.	0.2	15
13	The <scp>D</scp>alton quantum chemistry program system. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 269-284.	6.2	1,166
14	Photoabsorption of Acridine Yellow and Proflavin Bound to Human Serum Albumin Studied by Means of Quantum Mechanics/Molecular Dynamics. Journal of Physical Chemistry B, 2013, 117, 2069-2080.	1.2	18
15	A quantum mechanics/molecular dynamics study of electric field gradient fluctuations in the liquid phase. The case of Na⁺in aqueous solution. Physical Chemistry Chemical Physics, 2013, 15, 1621-1631.	1.3	16
16	NMR and Raman Spectroscopy Monitoring of Proton/Deuteron Exchange in Aqueous Solutions of Ionic Liquids Forming Hydrogen Bond: A Role of Anions, Self-Aggregation, and Mesophase Formation. Journal of Physical Chemistry B, 2013, 117, 10211-10220.	1.2	21
17	Amyloid Fibril-Induced Structural and Spectral Modifications in the Thioflavin-T Optical Probe. Journal of Physical Chemistry Letters, 2013, 4, 70-77.	2.1	29
18	Hydrogen Bonding in Pyridine N-Oxide/Acid Systems: Proton Transfer and Fine Details Revealed by FTIR, NMR, and X-ray Diffraction. Journal of Physical Chemistry A, 2012, 116, 8753-8761.	1.1	21

#	ARTICLE	IF	CITATIONS
19	NMR Spinâ€“Spin Coupling Constants in Polymethine Dyes as Polarity Indicators. Chemistry - A European Journal, 2012, 18, 11677-11684.	1.7	14
20	Hybrid density functional theory/molecular mechanics calculations of two-photon absorption of dimethylamino nitro stilbene in solution. Physical Chemistry Chemical Physics, 2011, 13, 12506.	1.3	64
21	Density Functional Theory/Molecular Mechanics Approach for Electronic g-Tensors of Solvated Molecules. Journal of Physical Chemistry B, 2011, 115, 4350-4358.	1.2	20
22	Excitation Energies in Solution: The Fully Polarizable QM/MM/PCM Method. Journal of Physical Chemistry B, 2011, 115, 3027-3037.	1.2	118
23	Fluorescence and phosphorescence of acetone in neat liquid and aqueous solution studied by QM/MM and PCM approaches. International Journal of Quantum Chemistry, 2011, 111, 1511-1520.	1.0	17
24	Computational protocols for prediction of solute NMR relative chemical shifts. A case study of <scp>L</scp>â€tryptophan in aqueous solution. Journal of Computational Chemistry, 2011, 32, 2853-2864.	1.5	25
25	Intramolecular soft modes and intermolecular interactions in liquid acetone. Physical Review B, 2011, 84, .	1.1	44
26	Excited States in Solution through Polarizable Embedding. Journal of Chemical Theory and Computation, 2010, 6, 3721-3734.	2.3	293
27	NMR and Quantum Chemistry Study of Mesoscopic Effects in Ionic Liquids. Journal of Physical Chemistry A, 2010, 114, 5365-5371.	1.1	31
28	Solvatochromic Shifts in Uracil: A Combined MD-QM/MM Study. Journal of Chemical Theory and Computation, 2010, 6, 249-256.	2.3	66
29	The Effect of Solvation on the Mean Excitation Energy of Glycine. Journal of Physical Chemistry Letters, 2010, 1, 242-245.	2.1	20
30	Modeling the Structure and Absorption Spectra of Stilbazolium Merocyanine in Polar and Nonpolar Solvents Using Hybrid QM/MM Techniques. Journal of Physical Chemistry B, 2010, 114, 13349-13357.	1.2	52
31	On the existence of the H3 tautomer of adenine in aqueous solution. Rationalizations based on hybrid quantum mechanics/molecular mechanics predictions. Physical Chemistry Chemical Physics, 2010, 12, 761-768.	1.3	25
32	Prediction of spin-spin coupling constants in solution based on combined density functional theory/molecular mechanics. Journal of Chemical Physics, 2009, 130, 134508.	1.2	48
33	NMR and DFT study on media effects on proton transfer in hydrogen bonding: concept of molecular probe with an application to ionic and super-polar liquids. Physical Chemistry Chemical Physics, 2009, 11, 8592.	1.3	17
34	Solvent effects on the nitrogen NMR shielding and nuclear quadrupole coupling constants in 1-methyltriazoles. Chemical Physics Letters, 2008, 460, 129-136.	1.2	16
35	On the Accuracy of Density Functional Theory to Predict Shifts in Nuclear Magnetic Resonance Shielding Constants due to Hydrogen Bonding. Journal of Chemical Theory and Computation, 2008, 4, 267-277.	2.3	51
36	On the performance of quantum chemical methods to predict solvatochromic effects: The case of acrolein in aqueous solution. Journal of Chemical Physics, 2008, 128, 194503.	1.2	76

#	ARTICLE	IF	CITATIONS
37	Modelling spectroscopic properties of large molecular systems. The combined Density Functional Theory/Molecular Mechanics approach. Journal of Computational Methods in Sciences and Engineering, 2008, 7, 135-158.	0.1	4
38	Linear Response Theory in Connection to Density Functional Theory/Molecular Dynamics and Coupled Cluster/Molecular Dynamics Methods. Challenges and Advances in Computational Chemistry and Physics, 2008, , 349-380.	0.6	2
39	Proton transfer in hydrogen-bonded pyridine/acid systems: the role of higher aggregation. Physical Chemistry Chemical Physics, 2007, 9, 3181.	1.3	29
40	Solvent Effects on NMR Isotropic Shielding Constants. A Comparison between Explicit Polarizable Discrete and Continuum Approaches. Journal of Physical Chemistry A, 2007, 111, 4199-4210.	1.1	74
41	Determination of Critical Indices by â€œSlowâ€•Spectroscopy:Â NMR Shifts by Statistical Thermodynamics and Density Functional Theory Calculations. Journal of Physical Chemistry B, 2007, 111, 2523-2532.	1.2	8
42	Gauge-origin independent magnetizabilities from hybrid quantum mechanics/molecular mechanics models: Theory and applications to liquid water. Chemical Physics Letters, 2007, 442, 322-328.	1.2	3
43	Temperature Dependence of 1H and 17O NMR Shifts of Water: Entropy Effect. Applied Magnetic Resonance, 2007, 32, 363-376.	0.6	12
44	A¹³C NMR and density functional theory study of critical behaviour of binary water/2,6-lutidine solution. Lithuanian Journal of Physics, 2007, 47, 443-449.	0.1	13
45	Proton transfer in H-bond: Possibility of short-range order solvent effect. Journal of Molecular Liquids, 2006, 127, 134-138.	2.3	10
46	Magnetic shielding properties of water in various molecular and molecular-ionic structures. Lithuanian Journal of Physics, 2006, 46, 169-175.	0.1	3
47	1H NMR and DFT study of proton exchange in heterogeneous structures of pyridine-N-oxide/HCl/DCl/H2O. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2005, 61, 835-839.	2.0	10
48	Coupled Cluster Calculation of the n â†' Ï€* Electronic Transition of Acetone in Aqueous Solution. Journal of Physical Chemistry A, 2005, 109, 8001-8010.	1.1	107