Miroslav Medved

List of Publications by Year
in descending order

77 papers	1,862 citations	279487 23 h-index	301761 39 g-index
78 all docs	78 docs citations	78 times ranked	2186 citing authors

#	Article	IF	Citations
1	First hyperpolarizability of polymethineimine with long-range corrected functionals. Journal of Chemical Physics, 2007, 126, 191108.	1.2	158
2	Mixedâ€Valence Singleâ€Atom Catalyst Derived from Functionalized Graphene. Advanced Materials, 2019, 31, e1900323.	11.1	129
3	Shedding Light on the Photoisomerization Pathway of Donorâ€“Acceptor Stenhouse Adducts. Journal of the American Chemical Society, 2017, 139, 15596-15599.	6.6	88
4	Solvent Effects on the Actinic Step of Donorâ€“Acceptor Stenhouse Adduct Photoswitching. Angewandte Chemie - International Edition, 2018, 57, 8063-8068.	7.2	70
5	Nonlinear Optical Properties of Ferrocene- and Porphyrinâ€“[60]Fullerene Dyads. ChemPhysChem, 2007, 8, 1056-1064.	1.0	64
6	Iminothioindoxyl as a molecular photoswitch with 100â€‰nm band separation in the visible range. Nature Communications, 2019, 10, 2390.	5.8	63
7	A generalized Romberg differentiation procedure for calculation of hyperpolarizabilities. Computational and Theoretical Chemistry, 2007, 847, 39-46.	1.5	59
8	Progress and challenges in understanding of photoluminescence properties of carbon dots based on theoretical computations. Applied Materials Today, 2021, 22, 100924.	2.3	57
9	Reactivity of fluorographene is triggered by point defects: beyond the perfect 2D world. Nanoscale, 2018, 10, 4696-4707.	2.8	55
10	Tailoring Photoisomerization Pathways in Donorâ€“Acceptor Stenhouse Adducts: The Role of the Hydroxy Group. Journal of Physical Chemistry A, 2018, 122, 955-964.	1.1	54
11	Nitrogen doped graphene with diamond-like bonds achieves unprecedented energy density at high power in a symmetric sustainable supercapacitor. Energy and Environmental Science, 2022, 15, 740-748.	15.6	51
12	Using Timeâ€Dependent Density Functional Theory to Probe the Nature of Donorâ€“Acceptor Stenhouse Adduct Photochromes. ChemPhysChem, 2016, 17, 1846-1851.	1.0	50
13	2D Chemistry: Chemical Control of Graphene Derivatization. Journal of Physical Chemistry Letters, 2018, 9, 3580-3585.	2.1	47
14	Benchmark calculations of some molecular properties of O2, CN and other selected small radicals using the ROHF-CCSD(T) method. Molecular Physics, 2002, 100, 541-560.	0.8	44
15	Tailoring Ï€-conjugation and vibrational modes to steer on-surface synthesis of pentalene-bridged ladder polymers. Nature Communications, 2020, 11, 4567.	5.8	36
16	Carbon Dots Detect Water-to-Ice Phase Transition and Act as Alcohol Sensors via Fluorescence Turn-Off/On Mechanism. ACS Nano, 2021, 15, 6582-6593.	7.3	34
17	Accuracy assessment of the ROHF â€” CCSD(T) calculations of static dipole polarizabilities of diatomic radicals: O2, CN, and NO. Computational and Theoretical Chemistry, 2001, 547, 219-232.	1.5	31
18	First-Principles Simulations of One- and Two-Photon Absorption Band Shapes of the Bis(BF₂) Core Complex. Journal of Physical Chemistry B, 2016, 120, 2323-2332.	1.2	28

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19	Covalently Interlinked Graphene Sheets with Sulfurâ€Chains Enable Superior Lithiumâ€“Sulfur Battery Cathodes at Fullâ€Mass Level. Advanced Functional Materials, 2021, 31, 2101326.	7.8	27
20	Tunable Synthesis of Nitrogen Doped Graphene from Fluorographene under Mild Conditions. ACS Sustainable Chemistry and Engineering, 2020, 8, 4764-4772.	3.2	26
21	Dipole moment and polarizability of the low-lying excited states of uracil. Chemical Physics Letters, 2012, 546, 24-29.	1.2	25
22	Intrinsic photoluminescence of amine-functionalized graphene derivatives for bioimaging applications. Applied Materials Today, 2019, 17, 112-122.	2.3	25
23	Conformational Behavior and Optical Properties of a Fluorophore Dimer as a Model of Luminescent Centers in Carbon Dots. Journal of Physical Chemistry C, 2020, 124, 14327-14337.	1.5	25
24	Molecular Fluorophores Self-Organize into C-Dot Seeds and Incorporate into C-Dot Structures. Journal of Physical Chemistry Letters, 2020, 11, 8252-8258.	2.1	24
25	Static NLO responses of fluorinated polyacetylene chains evaluated with long-range corrected density functionals. Chemical Physics Letters, 2011, 515, 78-84.	1.2	23
26	Solvatochromic Shifts in UVâ€“Vis Absorption Spectra: The Challenging Case of 4-Nitropyridine N-Oxide. Journal of Chemical Theory and Computation, 2016, 12, 1919-1929.	2.3	23
27	Alkynylation of graphene via the Sonogashira Câ€“C cross-coupling reaction on fluorographene. Chemical Communications, 2019, 55, 1088-1091.	2.2	23
28	Variability of Câ€“F Bonds Governs the Formation of Specific Structural Motifs in Fluorinated Graphenes. Journal of Physical Chemistry C, 2019, 123, 27896-27903.	1.5	22
29	Contribution of the Molecular Fluorophore IPCA to Excitation-Independent Photoluminescence of Carbon Dots. Journal of Physical Chemistry C, 2021, 125, 12140-12148.	1.5	22
30	CCSD(T) expectation value calculations of first-order properties. Theoretical Chemistry Accounts, 1997, 98, 75-84.	0.5	21
31	Solvent Effects on the Actinic Step of Donorâ€“Acceptor Stenhouse Adduct Photoswitching. Angewandte Chemie, 2018, 130, 8195-8200.	1.6	21
32	Can Density Functional Theory Be Trusted for High-Order Electric Properties? The Case of Hydrogen-Bonded Complexes. Journal of Chemical Theory and Computation, 2019, 15, 3570-3579.	2.3	21
33	Combined high degree of carboxylation and electronic conduction in graphene acid sets new limits for metal free catalysis in alcohol oxidation. Chemical Science, 2019, 10, 9438-9445.	3.7	20
34	Zigzag sp² Carbon Chains Passing through an sp³ Framework: A Driving Force toward Room-Temperature Ferromagnetic Graphene. ACS Nano, 2018, 12, 12847-12859.	7.3	19
35	Exploring the Solvatochromism of Betaineâ€…30 with Ab Initio Tools: From Accurate Gasâ€Phase Calculations to Implicit and Explicit Solvation Models. Chemistry - A European Journal, 2017, 23, 4108-4119.	1.7	18
36	Quantifying the Performances of DFT for Predicting Vibrationally Resolved Optical Spectra: Asymmetric Fluoroborate Dyes as Working Examples. Journal of Chemical Theory and Computation, 2017, 13, 4347-4356.	2.3	18

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37	On the physical origins of interaction-induced vibrational (hyper)polarizabilities. Physical Chemistry Chemical Physics, 2016, 18, 22467-22477.	1.3	16
38	Tunable one-step double functionalization of graphene based on fluorographene chemistry. Chemical Communications, 2020, 56, 1936-1939.	2.2	16
39	Thermally reduced fluorographenes as efficient electrode materials for supercapacitors. Nanoscale, 2019, 11, 21364-21375.	2.8	15
40	Linear phosphorus-boron chains: model system with huge electronic first hyperpolarizability. International Journal of Quantum Chemistry, 2005, 103, 226-234.	1.0	14
41	Comparison of Property-Oriented Basis Sets for the Computation of Electronic and Nuclear Relaxation Hyperpolarizabilities. Journal of Chemical Theory and Computation, 2015, 11, 4119-4128.	2.3	14
42	Full cLR-PCM calculations of the solvatochromic effects on emission energies. Physical Chemistry Chemical Physics, 2014, 16, 26024-26029.	1.3	13
43	Electric properties of the low-lying excited states of benzonitrile: geometry relaxation and solvent effects. Theoretical Chemistry Accounts, 2015, 134, 1.	0.5	13
44	Tailoring the optical and dynamic properties of iminothioindoxyl photoswitches through acidochromism. Chemical Science, 2021, 12, 4588-4598.	3.7	13
45	Effect of the leaving group on the reaction of 2-aminopyrroles with electron deficient heteroaromatic azadienes: substitution by additionâ€“elimination versus cycloaddition. Tetrahedron Letters, 2007, 48, 3991-3994.	0.7	12
46	Unveiling Solvents Effect on Excited-State Polarizabilities with the Corrected Linear-Response Model. Journal of Physical Chemistry A, 2014, 118, 5652-5656.	1.1	12
47	Direct and Indirect Effects of Dispersion Interactions on the Electric Properties of Weakly Bound Complexes. Journal of Physical Chemistry A, 2015, 119, 3112-3124.	1.1	12
48	Partitioning of interaction-induced nonlinear optical properties of molecular complexes. I. Hydrogen-bonded systems. Physical Chemistry Chemical Physics, 2018, 20, 19841-19849.	1.3	12
49	Bimodal role of fluorine atoms in fluorographene chemistry opens a simple way toward double functionalization of graphene. Carbon, 2019, 145, 251-258.	5.4	12
50	High second-order NLO responses of dehydrogenated hydrogen cyanide borane(1) oligomers. Computational and Theoretical Chemistry, 2010, 961, 66-72.	1.5	11
51	Theoretical analysis of charge-transfer electronic spectra of methylated benzenesâ€”TCNE complexes including solvent effects: approaching experiment. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	11
52	EFFECT OF ELECTRON-WITHDRAWING SUBSTITUENTS ON THE INVERSE-ELECTRON DEMAND DIELS-ALDER REACTION OF 2-AMINOPYRROLES AND 1,3,5-TRIAZINES. Heterocyclic Communications, 2007, 13, .	0.6	10
53	MP2, DFTâ€Ð, and PCM study of the HMBâ€“TCNE complex: Thermodynamics, electric properties, and solvent effects. International Journal of Quantum Chemistry, 2008, 108, 1533-1545.	1.0	10
54	Weakly interacting molecular clusters of CO with H₂O, SO₂, and NO⁺. Molecular Physics, 2014, 112, 3225-3236.	0.8	10

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55	Optical properties of V-shaped bis-coumarins: Ab initio insights. Computational and Theoretical Chemistry, 2016, 1076, 57-64.	1.1	10
56	A DFT study of H-isomerisation in alkoxy-, alkylperoxy- and alkyl radicals: Some implications for radical chain reactions in polymer systems. Polymer Degradation and Stability, 2011, 96, 660-669.	2.7	9
57	Tuning the NLO properties of polymethineimine chains by chemical substitution. Chemical Physics, 2013, 415, 196-206.	0.9	9
58	Critical analysis of spectral solvent shifts calculated by the contemporary PCM approaches of a representative series of charge-transfer complexes between tetracyanoethylene and methylated benzenes. Physical Chemistry Chemical Physics, 2015, 17, 17618-17627.	1.3	8
59	Singleâ€Atom Catalysis: Mixedâ€Valence Singleâ€Atom Catalyst Derived from Functionalized Graphene (Adv.) Tj ETQq1 1 0.784314 r	11.1	8
60	Partitioning of interaction-induced nonlinear optical properties of molecular complexes. II. Halogen-bonded systems. Physical Chemistry Chemical Physics, 2020, 22, 4225-4234.	1.3	8
61	Longitudinal NLO properties of C2H2, HCCF, and C2F2: Electron correlation and vibration effects. International Journal of Quantum Chemistry, 2005, 102, 209-223.	1.0	7
62	NLO responses of small polymethineimine oligomers: A CCSD(T) study. Computational and Theoretical Chemistry, 2007, 821, 160-165.	1.5	6
63	Accurate Nonlinear Optical Properties of Solvated para-Nitroaniline Predicted by an Electrostatic Discrete Local Field Approach. Journal of Physical Chemistry B, 2020, 124, 10195-10209.	1.2	6
64	Anchoring of Transition Metals to Graphene Derivatives as an Efficient Approach for Designing Singleâ€Atom Catalysts. Advanced Materials Interfaces, 2021, 8, 2001392.	1.9	6
65	Design of High-Performance Pyridine/Quinoline Hydrazone Photoswitches. Journal of Organic Chemistry, 2021, 86, 11633-11646.	1.7	6
66	Theoretical study (CC2, DFT and PCM) of charge transfer complexes between antithyroid thioamides and TCNE: electronic CT transitions. Journal of Molecular Modeling, 2014, 20, 2312.	0.8	5
67	MP2 and DFT study of IR spectra of TCNEâ€methylsubstituted benzene complexes: Is charge transfer important?. International Journal of Quantum Chemistry, 2010, 110, 1712-1728.	1.0	4
68	Enhancement of the second-order NLO responses of boronâ€“nitrogen oligomers by copolymerization with polyyne. Computational and Theoretical Chemistry, 2009, 901, 194-201.	1.5	4
69	Solvent Effects on Molecular Electric Properties. , 2017, , 741-794.		4
70	Electric properties of hydrated uracil: From micro- to macrohydration. Journal of Molecular Liquids, 2019, 275, 338-346.	2.3	4
71	Theoretical study of charge transfer complexes between antithyroid thioamides and TCNE: Thermodynamics of the complex formation. Computational and Theoretical Chemistry, 2015, 1051, 129-136.	1.1	3
72	The behavior of a paramagnetic system in electric and magnetic fields as exemplified by revisiting Li@B₁₀H₁₄. Physical Chemistry Chemical Physics, 2017, 19, 12229-12236.	1.3	2

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73	Electric Properties of Cyanoborane Isomers. Collection of Czechoslovak Chemical Communications, 2005, 70, 1055-1081.	1.0	2
74	Stretchâ€Healable Molecular Nanofibers. Advanced Theory and Simulations, 2020, 3, 2000094.	1.3	1
75	Solvent Effects on Molecular Electric Properties. , 2015, , 1-54.		1
76	Accessibility of Grafted Functional Groups Limits Reactivity of Covalent Graphene Derivatives. Applied Surface Science, 2022, , 153792.	3.1	1
77	Using Time-Dependent Density Functional Theory to Probe the Nature of Donor-Acceptor Stenhouse Adduct Photochromes. ChemPhysChem, 2016, 17, 1712-1712.	1.0	0