Miroslav Medved

List of Publications by Year in Descending Order

77 papers	1,305 citations	18 h-index	32 g-index
78 ext. papers	1,603 ext. citations	6.4 avg, IF	4.59 L-index

#	Paper	IF	Citations
77	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	35.4	4
76	Accessibility of Grafted Functional Groups Limits Reactivity of Covalent Graphene Derivatives. *Applied Surface Science*, **2022**, 153792	6.7	1
75	Progress and challenges in understanding of photoluminescence properties of carbon dots based on theoretical computations. *Applied Materials Today*, **2021**, 22, 100924	6.6	23
74	Carbon Dots Detect Water-to-Ice Phase Transition and Act as Alcohol Sensors Fluorescence Turn-Off/On Mechanism. *ACS Nano*, **2021**, 15, 6582-6593	16.7	14
73	Covalently Interlinked Graphene Sheets with Sulfur-Chains Enable Superior Lithium□Sulfur Battery Cathodes at Full-Mass Level. *Advanced Functional Materials*, **2021**, 31, 2101326	15.6	6
72	Contribution of the Molecular Fluorophore IPCA to Excitation-Independent Photoluminescence of Carbon Dots. *Journal of Physical Chemistry C*, **2021**, 125, 12140-12148	3.8	6
71	Design of High-Performance Pyridine/Quinoline Hydrazone Photoswitches. *Journal of Organic Chemistry*, **2021**, 86, 11633-11646	4.2	1
70	Anchoring of Transition Metals to Graphene Derivatives as an Efficient Approach for Designing Single-Atom Catalysts. *Advanced Materials Interfaces*, **2021**, 8, 2001392	4.6	5
69	Tailoring the optical and dynamic properties of iminothioindoxyl photoswitches through acidochromism. *Chemical Science*, **2021**, 12, 4588-4598	9.4	4
68	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	3.8	13
67	Partitioning of interaction-induced nonlinear optical properties of molecular complexes. II. Halogen-bonded systems. *Physical Chemistry Chemical Physics*, **2020**, 22, 4225-4234	3.6	2
66	Tunable Synthesis of Nitrogen Doped Graphene from Fluorographene under Mild Conditions. *ACS Sustainable Chemistry and Engineering*, **2020**, 8, 4764-4772	8.3	17
65	Tunable one-step double functionalization of graphene based on fluorographene chemistry. *Chemical Communications*, **2020**, 56, 1936-1939	5.8	8
64	Accurate Nonlinear Optical Properties of Solvated -Nitroaniline Predicted by an Electrostatic Discrete Local Field Approach. *Journal of Physical Chemistry B*, **2020**, 124, 10195-10209	3.4	3
63	Tailoring □conjugation and vibrational modes to steer on-surface synthesis of pentalene-bridged ladder polymers. *Nature Communications*, **2020**, 11, 4567	17.4	12
62	Molecular Fluorophores Self-Organize into C-Dot Seeds and Incorporate into C-Dot Structures. *Journal of Physical Chemistry Letters*, **2020**, 11, 8252-8258	6.4	9
61	Stretch-Healable Molecular Nanofibers. *Advanced Theory and Simulations*, **2020**, 3, 2000094	3.5	1

60	Variability of C–F Bonds Governs the Formation of Specific Structural Motifs in Fluorinated Graphenes. *Journal of Physical Chemistry C*, **2019**, 123, 27896-27903	3.8	13
59	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	9.4	13
58	Bimodal role of fluorine atoms in fluorographene chemistry opens a simple way toward double functionalization of graphene. *Carbon*, **2019**, 145, 251-258	10.4	6
57	Alkynylation of graphene via the Sonogashira C-C cross-coupling reaction on fluorographene. *Chemical Communications*, **2019**, 55, 1088-1091	5.8	15
56	Iminothioindoxyl as a molecular photoswitch with 100 nm band separation in the visible range. *Nature Communications*, **2019**, 10, 2390	17.4	34
55	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	6.4	11
54	Single-Atom Catalysis: Mixed-Valence Single-Atom Catalyst Derived from Functionalized Graphene (Adv. Mater. 17/2019). *Advanced Materials*, **2019**, 31, 1970125	24	5
53	Mixed-Valence Single-Atom Catalyst Derived from Functionalized Graphene. *Advanced Materials*, **2019**, 31, e1900323	24	76
52	Intrinsic photoluminescence of amine-functionalized graphene derivatives for bioimaging applications. *Applied Materials Today*, **2019**, 17, 112-122	6.6	17
51	Thermally reduced fluorographenes as efficient electrode materials for supercapacitors. *Nanoscale*, **2019**, 11, 21364-21375	7.7	10
50	Electric properties of hydrated uracil: From micro- to macrohydration. *Journal of Molecular Liquids*, **2019**, 275, 338-346	6	2
49	Reactivity of fluorographene is triggered by point defects: beyond the perfect 2D world. *Nanoscale*, **2018**, 10, 4696-4707	7.7	45
48	Tailoring Photoisomerization Pathways in Donor-Acceptor Stenhouse Adducts: The Role of the Hydroxy Group. *Journal of Physical Chemistry A*, **2018**, 122, 955-964	2.8	41
47	Partitioning of interaction-induced nonlinear optical properties of molecular complexes. I. Hydrogen-bonded systems. *Physical Chemistry Chemical Physics*, **2018**, 20, 19841-19849	3.6	9
46	2D Chemistry: Chemical Control of Graphene Derivatization. *Journal of Physical Chemistry Letters*, **2018**, 9, 3580-3585	6.4	34
45	Zigzag sp Carbon Chains Passing through an sp Framework: A Driving Force toward Room-Temperature Ferromagnetic Graphene. *ACS Nano*, **2018**, 12, 12847-12859	16.7	10
44	Solvent Effects on the Actinic Step of Donor-Acceptor Stenhouse Adduct Photoswitching. *Angewandte Chemie - International Edition*, **2018**, 57, 8063-8068	16.4	47
43	Solvent Effects on the Actinic Step of Donor–Acceptor Stenhouse Adduct Photoswitching. *Angewandte Chemie*, **2018**, 130, 8195-8200	3.6	14

42	Solvent Effects on Molecular Electric Properties **2017**, 741-794		4
41	The behavior of a paramagnetic system in electric and magnetic fields as exemplified by revisiting Li@BH. *Physical Chemistry Chemical Physics*, **2017**, 19, 12229-12236	3.6	2
40	Exploring the Solvatochromism of Betaine 30 with Ab Initio Tools: From Accurate Gas-Phase Calculations to Implicit and Explicit Solvation Models. *Chemistry - A European Journal*, **2017**, 23, 4108-4119	5.8	12
39	Shedding Light on the Photoisomerization Pathway of Donor-Acceptor Stenhouse Adducts. *Journal of the American Chemical Society*, **2017**, 139, 15596-15599	16.4	63
38	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	6.4	14
37	On the physical origins of interaction-induced vibrational (hyper)polarizabilities. *Physical Chemistry Chemical Physics*, **2016**, 18, 22467-77	3.6	10
36	Using Time-Dependent Density Functional Theory to Probe the Nature of Donor-Acceptor Stenhouse Adduct Photochromes. *ChemPhysChem*, **2016**, 17, 1846-51	3.2	41
35	First-Principles Simulations of One- and Two-Photon Absorption Band Shapes of the Bis(BF2) Core Complex. *Journal of Physical Chemistry B*, **2016**, 120, 2323-32	3.4	21
34	Solvatochromic Shifts in UV-Vis Absorption Spectra: The Challenging Case of 4-Nitropyridine N-Oxide. *Journal of Chemical Theory and Computation*, **2016**, 12, 1919-29	6.4	18
33	Optical properties of V-shaped bis-coumarins: Ab initio insights. *Computational and Theoretical Chemistry*, **2016**, 1076, 57-64	2	5
32	Using Time-Dependent Density Functional Theory to Probe the Nature of Donor-Acceptor Stenhouse Adduct Photochromes. *ChemPhysChem*, **2016**, 17, 1712-1712	3.2	
31	Direct and indirect effects of dispersion interactions on the electric properties of weakly bound complexes. *Journal of Physical Chemistry A*, **2015**, 119, 3112-24	2.8	11
30	Comparison of Property-Oriented Basis Sets for the Computation of Electronic and Nuclear Relaxation Hyperpolarizabilities. *Journal of Chemical Theory and Computation*, **2015**, 11, 4119-28	6.4	13
29	Theoretical study of charge transfer complexes between antithyroid thioamides and TCNE: Thermodynamics of the complex formation. *Computational and Theoretical Chemistry*, **2015**, 1051, 129-136	2	3
28	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, 17618-27	3.6	8
27	Electric properties of the low-lying excited states of benzonitrile: geometry relaxation and solvent effects. *Theoretical Chemistry Accounts*, **2015**, 134, 1	1.9	11
26	Solvent Effects on Molecular Electric Properties **2015**, 1-54		0
25	Full cLR-PCM calculations of the solvatochromic effects on emission energies. *Physical Chemistry Chemical Physics*, **2014**, 16, 26024-9	3.6	11

24	Unveiling solvents effect on excited-state polarizabilities with the corrected linear-response model. *Journal of Physical Chemistry A*, **2014**, 118, 5652-6	2.8	11
23	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	2	4
22	Weakly interacting molecular clusters of CO with H2O, SO2, and NO+. *Molecular Physics*, **2014**, 112, 3225-3236	1.7	7
21	Tuning the NLO properties of polymethineimine chains by chemical substitution. *Chemical Physics*, **2013**, 415, 196-206	2.3	8
20	Dipole moment and polarizability of the low-lying excited states of uracil. *Chemical Physics Letters*, **2012**, 546, 24-29	2.5	25
19	Theoretical analysis of charge-transfer electronic spectra of methylated benzenes–TCNE complexes including solvent effects: approaching experiment. *Theoretical Chemistry Accounts*, **2012**, 131, 1	1.9	11
18	Static NLO responses of fluorinated polyacetylene chains evaluated with long-range corrected density functionals. *Chemical Physics Letters*, **2011**, 515, 78-84	2.5	23
17	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	4.7	7
16	High second-order NLO responses of dehydrogenated hydrogen cyanide borane(1) oligomers. *Computational and Theoretical Chemistry*, **2010**, 961, 66-72		9
15	MP2 and DFT study of IR spectra of TCNE-methylsubstituted benzene complexes: Is charge transfer important?. *International Journal of Quantum Chemistry*, **2009**, 110, NA-NA	2.1	2
14	Enhancement of the second-order NLO responses of boron–nitrogen oligomers by copolymerization with polyyne. *Computational and Theoretical Chemistry*, **2009**, 901, 194-201		4
13	MP2, DFT-D, and PCM study of the HMB–TCNE complex: Thermodynamics, electric properties, and solvent effects. *International Journal of Quantum Chemistry*, **2008**, 108, 1533-1545	2.1	10
12	Nonlinear optical properties of ferrocene- and porphyrin-[60]fullerene dyads. *ChemPhysChem*, **2007**, 8, 1056-64	3.2	62
11	Effect of the leaving group on the reaction of 2-aminopyrroles with electron deficient heteroaromatic azadienes: substitution by addition–elimination versus cycloaddition. *Tetrahedron Letters*, **2007**, 48, 3991-3994	2	12
10	NLO responses of small polymethineimine oligomers: A CCSD(T) study. *Computational and Theoretical Chemistry*, **2007**, 821, 160-165		6
9	A generalized Romberg differentiation procedure for calculation of hyperpolarizabilities. *Computational and Theoretical Chemistry*, **2007**, 847, 39-46		54
8	First hyperpolarizability of polymethineimine with long-range corrected functionals. *Journal of Chemical Physics*, **2007**, 126, 191108	3.9	151
7	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,	1.7	8

6	Longitudinal NLO properties of C2H2, HCCF, and C2F2: Electron correlation and vibration effects. *International Journal of Quantum Chemistry*, **2005**, 102, 209-223	2.1	7
5	Linear phosphorus–boron chains: model system with huge electronic first hyperpolarizability. *International Journal of Quantum Chemistry*, **2005**, 103, 226-234	2.1	14
4	Electric Properties of Cyanoborane Isomers. *Collection of Czechoslovak Chemical Communications*, **2005**, 70, 1055-1081		2
3	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	1.7	41
2	Accuracy assessment of the ROHF/CCSD(T) calculations of static dipole polarizabilities of diatomic radicals: O2, CN, and NO. *Computational and Theoretical Chemistry*, **2001**, 547, 219-232		28
1	CCSD(T) expectation value calculations of first-order properties. *Theoretical Chemistry Accounts*, **1997**, 98, 75-84	1.9	20