S Knippenberg

List of Publications by Year
in descending order

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44 papers	901 citations	394286 19 h-index	477173 29 g-index
44 all docs	44 docs citations	44 times ranked	970 citing authors

#	Article	IF	Citations
1	Exhibiting environment sensitive optical properties through multiscale modelling: A study of photoactivatable probes. Journal of Photochemistry and Photobiology A: Chemistry, 2022, 425, 113672.	2.0	2
2	The influence of lipid membranes on fluorescent probes' optical properties. Biochimica Et Biophysica Acta - Biomembranes, 2021, 1863, 183494.	1.4	11
3	Multiscale Simulations of Polyzwitterions in Aqueous Bulk Solutions and Brush Array Configurations. Soft Matter, 2021, , .	1.2	8
4	Cyanine dyes with tail length asymmetry enhance photoselection: AÂmultiscale study on DiD probes in a liquid disordered membrane. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2020, 224, 117329.	2.0	8
5	Photoisomerization of DiD: Molecular Dynamics Calculations Reveal the Influence of Tail Lengths. Journal of Physical Chemistry C, 2020, 124, 5829-5837.	1.5	1
6	Push/Pull Effect as Driving Force for Different Optical Responses of Azobenzene in a Biological Environment. Journal of Physical Chemistry C, 2020, 124, 8310-8322.	1.5	11
7	Influence of Membrane Phase on the Optical Properties of DPH. Molecules, 2020, 25, 4264.	1.7	4
8	Conformational Changes as Driving Force for Phase Recognition: The Case of Laurdan. Langmuir, 2019, 35, 11471-11481.	1.6	21
9	Orientational distribution of DPH in lipid membranes: a comparison of molecular dynamics calculations and experimental time-resolved anisotropy experiments. Physical Chemistry Chemical Physics, 2019, 21, 7594-7604.	1.3	13
10	Laurdan as a Molecular Rotor in Biological Environments. ACS Applied Bio Materials, 2019, 2, 5769-5778.	2.3	10
11	Environmental effects on the charge transfer properties of Graphene quantum dot based interfaces. International Journal of Quantum Chemistry, 2019, 119, e25882.	1.0	8
12	Combining (Non)linear Optical and Fluorescence Analysis of DiD To Enhance Lipid Phase Recognition. Journal of Chemical Theory and Computation, 2018, 14, 5350-5359.	2.3	11
13	Atomistic Picture of Fluorescent Probes with Hydrocarbon Tails in Lipid Bilayer Membranes: An Investigation of Selective Affinities and Fluorescent Anisotropies in Different Environmental Phases. Langmuir, 2018, 34, 9072-9084.	1.6	15
14	Triggering On/Off States of Photoswitchable Probes in Biological Environments. Journal of the American Chemical Society, 2017, 139, 4418-4428.	6.6	20
15	Benchmarking Post-Hartreeâ€“Fock Methods To Describe the Nonlinear Optical Properties of Polymethines: An Investigation of the Accuracy of Algebraic Diagrammatic Construction (ADC) Approaches. Journal of Chemical Theory and Computation, 2016, 12, 5465-5476.	2.3	13
16	Investigation into Biological Environments through (Non)linear Optics: A Multiscale Study of Laurdan Derivatives. Journal of Chemical Theory and Computation, 2016, 12, 6169-6181.	2.3	25
17	A Blue-Light-Emitting BODIPY Probe for Lipid Membranes. Langmuir, 2016, 32, 3495-3505.	1.6	34
18	Strong Electronic Coupling Dominates the Absorption and Fluorescence Spectra of Covalently Bound BisBODIPYs. Journal of Physical Chemistry A, 2015, 119, 1323-1331.	1.1	25

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19	Self-assembly and hybridization mechanisms of DNA with cationic polythiophene. Soft Matter, 2015, 11, 6460-6471.	1.2	24
20	The cage fragmentation of doubly ionized norbornane: A Born-Oppenheimer molecular dynamics study. Chemical Physics Letters, 2013, 584, 24-29.	1.2	3
21	Synthesis and Optical Properties of Pyrrolo[3,2-b]pyrrole-2,5(1H,4H)-dione (iDPP)-Based Molecules. Journal of Physical Chemistry A, 2013, 117, 2782-2789.	1.1	26
22	The Molecular Mechanism of Photochromism in Photo-Enolizable Quinoline and Napthyridine Derivatives. Journal of Physical Chemistry A, 2012, 116, 12321-12329.	1.1	2
23	Calculations of nonlinear response properties using the intermediate state representation and the algebraic-diagrammatic construction polarization propagator approach: Two-photon absorption spectra. Journal of Chemical Physics, 2012, 136, 064107.	1.2	68
24	Computational design of improved twoâ€photon active caging compounds based on nitrodibenzofuran. Journal of Computational Chemistry, 2012, 33, 1797-1805.	1.5	11
25	The band 12 issue of norbornane: A study of higher shake-up states. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 88, 102-110.	2.0	6
26	Large Amplitude Motions in Cyclopentene and 1-Butene: Quantum Chemical Insights into the Ground- and Excited State Potential Energy Surfaces. Zeitschrift Fur Physikalische Chemie, 2011, 225, 525-539.	1.4	1
27	The conformational stability of gaseous 1-butene studied by femtosecond nonlinear spectroscopy and ab initio calculations. Vibrational Spectroscopy, 2011, 56, 13-18.	1.2	13
28	Simulation of Photoelectron Spectra Using the Reflection Principle in Combination with Unrestricted Excitation ADC(2) to Assess the Accuracy of Excitedâ€State Calculations. ChemPhysChem, 2011, 12, 3180-3191.	1.0	9
29	Ring-puckering motion in cyclopentene studied by time-resolved rotational coherence spectroscopy and ab initio calculations. Physical Chemistry Chemical Physics, 2010, 12, 8190.	1.3	5
30	Correlation effects in the valence ionization spectra of large conjugated molecules: p-Benzoquinone, anthracenequinone and pentacenequinone. Journal of Electron Spectroscopy and Related Phenomena, 2010, 178-179, 61-79.	0.8	10
31	Probing electron correlation and nuclear dynamics in Momentum Space. Journal of Physics: Conference Series, 2010, 212, 012020.	0.3	8
32	Quantum Chemical Study of Conformational Fingerprints in the Photoelectron Spectra and (e, 2e) Electron Momentum Distributions ofn-Hexane. Journal of Physical Chemistry A, 2010, 114, 4400-4417.	1.1	33
33	The low-lying excited states of neutral polyacenes and their radical cations: a quantum chemical study employing the algebraic diagrammatic construction scheme of second order. Molecular Physics, 2010, 108, 2801-2813.	0.8	46
34	High resolution electron momentum spectroscopy of the valence orbitals of water. Chemical Physics, 2008, 343, 19-30.	0.9	70
35	Probing molecular conformations in momentum space: The case of n-pentane. Journal of Chemical Physics, 2007, 127, 174306.	1.2	34
36	Imaging Momentum Orbital Densities of Conformationally Versatile Molecules:Â A Benchmark Theoretical Study of the Molecular and Electronic Structures of Dimethoxymethane. Journal of Physical Chemistry A, 2007, 111, 5879-5897.	1.1	39

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37	Theoretical Study of the Fragmentation Pathways of Norbornane in Its Doubly Ionized Ground State. Journal of Physical Chemistry A, 2007, 111, 10834-10848.	1.1	13
38	Study of the molecular structure, ionization spectrum, and electronic wave function of 1,3-butadiene using electron momentum spectroscopy and benchmark Dyson orbital theories. Journal of Chemical Physics, 2006, 125, 104309.	1.2	56
39	Probing Dyson orbitals with Greenâ€™s Function theory and Electron Momentum Spectroscopy. Chemical Physics Letters, 2006, 421, 52-57.	1.2	45
40	Green's function study of the one-electron and shake-up ionization spectra of unsaturated hydrocarbon cage compounds. Journal of Computational Chemistry, 2006, 27, 1703-1722.	1.5	21
41	Probing the Shape and Stereochemistry of Molecular Orbitals in Locally Flexible Aromatic Chains:â€‰ A Penning Ionization Electron Spectroscopy and Green's Function Study of the Electronic Structure of Biphenyl. Journal of Physical Chemistry A, 2005, 109, 10535-10546.	1.1	28
42	The Band 12 Issue in the Electron Momentum Spectra of Norbornane: A Comparison with Additional Green's Function Calculations and Ultraviolet Photoemission Measurements. Journal of Physical Chemistry A, 2005, 109, 4267-4273.	1.1	19
43	Investigation into the Valence Electronic Structure of Norbornene Using Electron Momentum Spectroscopy, Green's Function, and Density Functional Theories. Journal of Physical Chemistry A, 2005, 109, 9324-9340.	1.1	28
44	Norbornane: An investigation into its valence electronic structure using electron momentum spectroscopy, and density functional and Greenâ€™s function theories. Journal of Chemical Physics, 2004, 121, 10525-10541.	1.2	43