# S Knippenberg

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/4562993/publications.pdf

Version: 2024-02-01

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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 | High resolution electron momentum spectroscopy of the valence orbitals of water. Chemical Physics, 2008, 343, 19-30. | 0.9 | 70 |
| 2 | 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 |
| 3 | 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 |
| 4 | 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 |
| 5 | Probing Dyson orbitals with Greenâ€™s Function theory and Electron Momentum Spectroscopy. Chemical Physics Letters, 2006, 421, 52-57. | 1.2 | 45 |
| 6 | 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 |
| 7 | 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 |
| 8 | Probing molecular conformations in momentum space: The case of n-pentane. Journal of Chemical Physics, 2007, 127, 174306. | 1.2 | 34 |
| 9 | A Blue-Light-Emitting BODIPY Probe for Lipid Membranes. Langmuir, 2016, 32, 3495-3505. | 1.6 | 34 |
| 10 | 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 |
| 11 | 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 |
| 12 | 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 |
| 13 | 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 |
| 14 | 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 |
| 15 | 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 |
| 16 | Self-assembly and hybridization mechanisms of DNA with cationic polythiophene. Soft Matter, 2015, 11, 6460-6471. | 1.2 | 24 |
| 17 | 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 |
| 18 | Conformational Changes as Driving Force for Phase Recognition: The Case of Laurdan. Langmuir, 2019, 35, 11471-11481. | 1.6 | 21 |

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|---|---|---|---|
| 19 | Triggering On/Off States of Photoswitchable Probes in Biological Environments. Journal of the American Chemical Society, 2017, 139, 4418-4428. | 6.6 | 20 |
| 20 | 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 |
| 21 | 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 |
| 22 | 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 |
| 23 | 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 |
| 24 | 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 |
| 25 | 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 |
| 26 | Computational design of improved twoâ€photon active caging compounds based on nitrodibenzofuran. Journal of Computational Chemistry, 2012, 33, 1797-1805. | 1.5 | 11 |
| 27 | 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 |
| 28 | 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 |
| 29 | The influence of lipid membranes on fluorescent probes' optical properties. Biochimica Et Biophysica Acta - Biomembranes, 2021, 1863, 183494. | 1.4 | 11 |
| 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 | Laurdan as a Molecular Rotor in Biological Environments. ACS Applied Bio Materials, 2019, 2, 5769-5778. | 2.3 | 10 |
| 32 | 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 |
| 33 | Probing electron correlation and nuclear dynamics in Momentum Space. Journal of Physics: Conference Series, 2010, 212, 012020. | 0.3 | 8 |
| 34 | Environmental effects on the charge transfer properties of Graphene quantum dot based interfaces. International Journal of Quantum Chemistry, 2019, 119, e25882. | 1.0 | 8 |
| 35 | 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 |
| 36 | Multiscale Simulations of Polyzwitterions in Aqueous Bulk Solutions and Brush Array Configurations. Soft Matter, 2021, , . | 1.2 | 8 |

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| 37 | 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 |
| 38 | 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 |
| 39 | Influence of Membrane Phase on the Optical Properties of DPH. Molecules, 2020, 25, 4264. | 1.7 | 4 |
| 40 | The cage fragmentation of doubly ionized norbornane: A Born-Oppenheimer molecular dynamics study. Chemical Physics Letters, 2013, 584, 24-29. | 1.2 | 3 |
| 41 | The Molecular Mechanism of Photochromism in Photo-Enolizable Quinoline and Napthyridine Derivatives. Journal of Physical Chemistry A, 2012, 116, 12321-12329. | 1.1 | 2 |
| 42 | 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 |
| 43 | 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 |
| 44 | Photoisomerization of DiD: Molecular Dynamics Calculations Reveal the Influence of Tail Lengths. Journal of Physical Chemistry C, 2020, 124, 5829-5837. | 1.5 | 1 |