# Hans Lischka

List of Publications by Year
in descending order

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|---|---|---|---|
| 315 papers | 16,575 citations | 14614 66 h-index | 20900 115 g-index |
| 323 all docs | 323 docs citations | 323 times ranked | 10247 citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Spin-density calculation via the graphical unitary group approach. Molecular Physics, 2023, 121, . | 0.8 | 3 |
| 2 | Pathways to fluorescence via restriction of intramolecular motion in substituted tetraphenylethylenes. Physical Chemistry Chemical Physics, 2022, 24, 1722-1735. | 1.3 | 8 |
| 3 | Excitonic and charge transfer interactions in tetracene stacked and T-shaped dimers. Journal of Chemical Physics, 2021, 154, 044306. | 1.2 | 11 |
| 4 | Triple-Columned and Multiple-Layered 3D Polymers: Design, Synthesis, Aggregation-Induced Emission (AIE), and Computational Study. Research, 2021, 2021, 3565791. | 2.8 | 10 |
| 5 | A general new method for calculating the molecular nonpolar surface for analysis of LC-MS data. International Journal of Mass Spectrometry, 2021, 461, 116495. | 0.7 | 3 |
| 6 | Progress and challenges in understanding of photoluminescence properties of carbon dots based on theoretical computations. Applied Materials Today, 2021, 22, 100924. | 2.3 | 57 |
| 7 | Reaction mechanism for fluorination reactions with hydroxylated alumina sites: Pathways promoting aluminum combustion. Journal of Chemical Physics, 2021, 154, 104308. | 1.2 | 2 |
| 8 | Molecular Dynamics Simulation of the Excited-State Proton Transfer Mechanism in 3-Hydroxyflavone Using Explicit Hydration Models. Journal of Physical Chemistry A, 2021, 125, 5765-5778. | 1.1 | 10 |
| 9 | Ab initio calculation of the excited states of nitropyrenes. Theoretical Chemistry Accounts, 2021, 140, 1. | 0.5 | 2 |
| 10 | Unexpected Charge Effects Strengthen Ï€â€“Stacking Pancake Bonding. Jacs Au, 2021, 1, 1647-1655. | 3.6 | 15 |
| 11 | Exploration of Graphene Defect Reactivity toward a Hydrogen Radical Utilizing a Preactivated Circumcoronene Model. Journal of Physical Chemistry A, 2021, 125, 1152-1165. | 1.1 | 10 |
| 12 | Adsorption process of polar and nonpolar compounds in a nanopore model of humic substances. European Journal of Soil Science, 2020, 71, 845-855. | 1.8 | 11 |
| 13 | Dynamics of Pyrene-Dimer Association and Ensuing Pyrene-Dimer Dissociation. Journal of Physical Chemistry A, 2020, 124, 8907-8917. | 1.1 | 17 |
| 14 | Cycloaddition of Strained Cyclic Alkenes and Ortho-Quinones: A Distortion/Interaction Analysis. Journal of Organic Chemistry, 2020, 85, 13557-13566. | 1.7 | 8 |
| 15 | Tuning the UV spectrum of PAHs by means of different N-doping types taking pyrene as paradigmatic example: categorizationviavalence bond theory and high-level computational approaches. Physical Chemistry Chemical Physics, 2020, 22, 22003-22015. | 1.3 | 10 |
| 16 | Doping Capabilities of Fluorine on the UV Absorption and Emission Spectra of Pyrene-Based Graphene Quantum Dots. Journal of Physical Chemistry A, 2020, 124, 10954-10966. | 1.1 | 9 |
| 17 | Energy transfer mechanism in luminescence Eu(III) and Tb(III) complexes of coumarin-3-carboxylic acid: A theoretical study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2020, 240, 118591. | 2.0 | 12 |
| 18 | Effects on the aromaticity and on the biradicaloid nature of acenes by the inclusion of a cyclobutadiene linkage. Theoretical Chemistry Accounts, 2020, 139, 1. | 0.5 | 5 |

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| 19 | 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 |
| 20 | A computational study of the ground and excited state acidities of synthetic analogs of red wine pyranoanthocyanins. Theoretical Chemistry Accounts, 2020, 139, 1. | 0.5 | 9 |
| 21 | Diradical Organic Oneâ€Dimensional Polymers Synthesized on a Metallic Surface. Angewandte Chemie, 2020, 132, 17747-17752. | 1.6 | 14 |
| 22 | Memorial Viewpoint for William L. Hase. Journal of Physical Chemistry A, 2020, 124, 4183-4184. | 1.1 | 0 |
| 23 | Diradical Organic Oneâ€Dimensional Polymers Synthesized on a Metallic Surface. Angewandte Chemie - International Edition, 2020, 59, 17594-17599. | 7.2 | 33 |
| 24 | Interplay of Biradicaloid Character and Singlet/Triplet Energy Splitting for cis-/trans-Diindenoacenes and Related Benzothiophene-Capped Oligomers as Revealed by Extended Multireference Calculations. Journal of Organic Chemistry, 2020, 85, 3664-3675. | 1.7 | 16 |
| 25 | Benchmark ab initio calculations on intermolecular structures and the exciton character of poly(p-phenylenevinylene) dimers. Journal of Chemical Physics, 2020, 152, 044306. | 1.2 | 5 |
| 26 | The generality of the GUGA MRCI approach in COLUMBUS for treating complex quantum chemistry. Journal of Chemical Physics, 2020, 152, 134110. | 1.2 | 42 |
| 27 | Multi-layer 3D chirality: new synthesis, AIE and computational studies. Science China Chemistry, 2020, 63, 692-698. | 4.2 | 27 |
| 28 | A systematic analysis of excitonic properties to seek optimal singlet fission: the BN-substitution patterns in tetracene. Journal of Materials Chemistry C, 2020, 8, 7793-7804. | 2.7 | 22 |
| 29 | Nonadiabatic Dynamics of Charge-Transfer States Using the Anthraceneâ€“Tetracyanoethylene Complex as a Prototype. Journal of Physical Chemistry A, 2020, 124, 3347-3357. | 1.1 | 13 |
| 30 | Theoretical analysis of the stabilization of graphene nanosheets by means of strongly polarized pyrene derivatives. Chemical Physics, 2019, 527, 110468. | 0.9 | 5 |
| 31 | Characterization of glycan isomers using magnetic carbon nanoparticles as a MALDI co-matrix. RSC Advances, 2019, 9, 20137-20148. | 1.7 | 13 |
| 32 | Microhydration of Polymer Electrolyte Membranes: A Comparison of Hydrogen-Bonding Networks and Spectral Properties of Nafion and Bis[(perfluoroalkyl)sulfonyl] Imide. Journal of Physical Chemistry B, 2019, 123, 9899-9911. | 1.2 | 3 |
| 33 | Emission Energies and Stokes Shifts for Single Polycyclic Aromatic Hydrocarbon Sheets in Comparison to the Effect of Excimer Formation. Journal of Physical Chemistry Letters, 2019, 10, 5592-5597. | 2.1 | 18 |
| 34 | The electronic transitions of analogs of red wine pyranoanthocyanin pigments. Photochemical and Photobiological Sciences, 2019, 18, 45-53. | 1.6 | 16 |
| 35 | The characterization of electronic defect states of single and double carbon vacancies in graphene sheets using molecular density functional theory. Molecular Physics, 2019, 117, 1519-1531. | 0.8 | 10 |
| 36 | Solvent effect on Al(III) hydrolysis constants from density functional theory. Molecular Physics, 2019, 117, 1507-1518. | 0.8 | 0 |

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| 37 | Dynamics of benzene excimer formation from the parallel-displaced dimer. Physical Chemistry Chemical Physics, 2019, 21, 13916-13924. | 1.3 | 23 |
| 38 | Conical intersections and the weak fluorescence of betalains. Photochemical and Photobiological Sciences, 2019, 18, 1972-1981. | 1.6 | 3 |
| 39 | Introduction of polar or nonpolar groups at the hydroquinone units can lead to the destruction of the columnar structure of Pillar[5]arenes. Computational and Theoretical Chemistry, 2019, 1161, 1-9. | 1.1 | 11 |
| 40 | Characterization of Charge Transfer in Excited States of Extended Clusters of Ï€-Stacked Donor and Acceptor Complexes in Lock-Arm Supramolecular Ordering. Journal of Physical Chemistry A, 2019, 123, 4532-4542. | 1.1 | 7 |
| 41 | Quantum chemical evidence for the origin of the red/blue colors of Hydrangea macrophylla sepals. New Journal of Chemistry, 2019, 43, 7532-7540. | 1.4 | 7 |
| 42 | Excited states and excitonic interactions in prototypic polycyclic aromatic hydrocarbon dimers as models for graphitic interactions in carbon dots. Physical Chemistry Chemical Physics, 2019, 21, 9077-9088. | 1.3 | 34 |
| 43 | High-level theoretical benchmark investigations of the UV-vis absorption spectra of paradigmatic polycyclic aromatic hydrocarbons as models for graphene quantum dots. Journal of Chemical Physics, 2019, 150, 124302. | 1.2 | 35 |
| 44 | A Multireference Ab Initio Study of the Diradical Isomers of Pyrazine. Journal of Physical Chemistry A, 2019, 123, 2049-2057. | 1.1 | 9 |
| 45 | Kinetics of the Strain-Promoted Oxidation-Controlled Cycloalkyne-1,2-quinone Cycloaddition: Experimental and Theoretical Studies. Journal of Organic Chemistry, 2018, 83, 244-252. | 1.7 | 24 |
| 46 | The crucial role of a spacer material on the efficiency of charge transfer processes in organic donorâ€“acceptor junction solar cells. Nanoscale, 2018, 10, 451-459. | 2.8 | 5 |
| 47 | Analysis of charge transfer transitions in stacked Ï€-electron donorâ€“acceptor complexes. Physical Chemistry Chemical Physics, 2018, 20, 26957-26967. | 1.3 | 19 |
| 48 | Electronic structure theory gives insights into the higher efficiency of the PTB electron-donor polymers for organic photovoltaics in comparison with prototypical P3HT. Journal of Chemical Physics, 2018, 149, 184905. | 1.2 | 2 |
| 49 | Interplay between Aromaticity and Radicaloid Character in Nitrogen-Doped Oligoacenes Revealed by High-Level Multireference Methods. Journal of Physical Chemistry A, 2018, 122, 9464-9473. | 1.1 | 6 |
| 50 | The effect of hydrogen bonding on the nonadiabatic dynamics of a thymine-water cluster. Chemical Physics, 2018, 515, 472-479. | 0.9 | 13 |
| 51 | Multireference Approaches for Excited States of Molecules. Chemical Reviews, 2018, 118, 7293-7361. | 23.0 | 287 |
| 52 | Tuning the Biradicaloid Nature of Polycyclic Aromatic Hydrocarbons: The Effect of Graphitic Nitrogen Doping in Zethrenes. ChemPhysChem, 2018, 19, 2492-2499. | 1.0 | 11 |
| 53 | Model Systems for Dynamics of Ï€-Conjugated Biomolecules in Excited States. , 2017, , 1697-1739. | | 1 |
| 54 | Cationâ€“Ï€ interactions in competition with cation microhydration: a theoretical study of alkali metal cationâ€“pyrene complexes. Journal of Molecular Modeling, 2017, 23, 131. | 0.8 | 12 |

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| 55 | Local Electron Correlation Treatment in Extended Multireference Calculations: Effect of Acceptorâ€"Donor Substituents on the Biradical Character of the Polycyclic Aromatic Hydrocarbon Heptazethrene. Journal of Chemical Theory and Computation, 2017, 13, 2612-2622. | 2.3 | 13 |
| 56 | Highâ€level Ab Initio Absorption Spectra Simulations of Neutral, Anionic and Neutral+ Chromophore of Green Fluorescence Protein Chromophore Models in Gas Phase and Solution. Photochemistry and Photobiology, 2017, 93, 1356-1367. | 1.3 | 4 |
| 57 | Evaluation of the quasi correlated tight-binding (QCTB) model for describing polyradical character in polycyclic hydrocarbons. Journal of Chemical Physics, 2017, 146, 064106. | 1.2 | 21 |
| 58 | <scp>L</scp>agrange function method for energy optimization directly in the space of natural orbitals. International Journal of Quantum Chemistry, 2017, 117, e25376. | 1.0 | 3 |
| 59 | Investigation of the ozone formation reaction pathway: Comparisons of full configuration interaction quantum Monte Carlo and fixed-node diffusion Monte Carlo with contracted and uncontracted MRCI. Journal of Chemical Physics, 2017, 147, 094306. | 1.2 | 10 |
| 60 | Singlet L<sub>a</sub> and L<sub>b</sub> Bands for N-Acenes (N = 2â€"7): A CASSCF/CASPT2 Study. Journal of Chemical Theory and Computation, 2017, 13, 4297-4306. | 2.3 | 30 |
| 61 | Structure and electronic states of a graphene double vacancy with an embedded Si dopant. Journal of Chemical Physics, 2017, 147, 194702. | 1.2 | 9 |
| 62 | How to efficiently tune the biradicaloid nature of acenes by chemical doping with boron and nitrogen. Physical Chemistry Chemical Physics, 2017, 19, 19225-19233. | 1.3 | 23 |
| 63 | Single and double carbon vacancies in pyrene as first models for graphene defects: A survey of the chemical reactivity toward hydrogen. Chemical Physics, 2017, 482, 346-354. | 0.9 | 9 |
| 64 | New Insights into the State Trapping of UV-Excited Thymine. Molecules, 2016, 21, 1603. | 1.7 | 31 |
| 65 | The Antiferromagnetic Spin Coupling in Nonâ€KekulÃ© Acenesâ€"Impressive Polyradical Character Revealed by Highâ€Level Multireference Methods. ChemPhysChem, 2016, 17, 2013-2021. | 1.0 | 4 |
| 66 | <scp>Molcas</scp> 8: New capabilities for multiconfigurational quantum chemical calculations across the periodic table. Journal of Computational Chemistry, 2016, 37, 506-541. | 1.5 | 1,317 |
| 67 | Insight into the Excited State Electronic and Structural Properties of the Organic Photovoltaic Donor Polymer Poly(thieno[3,4-b]thiophene benzodithiophene) by Means of ab Initio and Density Functional Theory. Journal of Physical Chemistry C, 2016, 120, 21818-21826. | 1.5 | 22 |
| 68 | Ï€â€"Ï€ stacking between polyaromatic hydrocarbon sheets beyond dispersion interactions. Physical Chemistry Chemical Physics, 2016, 18, 22300-22310. | 1.3 | 57 |
| 69 | Polyradical Character of Triangular Non-KekulÃ© Structures, Zethrenes, p-Quinodimethane-Linked Bisphenalenyl, and the Clar Goblet in Comparison: An Extended Multireference Study. Journal of Physical Chemistry A, 2016, 120, 1625-1636. | 1.1 | 91 |
| 70 | Model Systems for Dynamics of Ï€-Conjugated Biomolecules in Excited States. , 2016, , 1-43. | | 0 |
| 71 | Intramolecular Charge-Transfer Excited-State Processes in 4-(N,N-Dimethylamino)benzonitrile: The Role of Twisting and the Ï€Ïƒ* State. Journal of Physical Chemistry A, 2015, 119, 6232-6243. | 1.1 | 60 |
| 72 | Why water makes 2-aminopurine fluorescent?. Physical Chemistry Chemical Physics, 2015, 17, 15452-15459. | 1.3 | 28 |

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| 73 | Absorption and Fluorescence Spectra of Poly(p-phenylenevinylene) (PPV) Oligomers: An ab Initio Simulation. Journal of Physical Chemistry A, 2015, 119, 1787-1795. | 1.1 | 22 |
| 74 | The electronic states of a double carbon vacancy defect in pyrene: a model study for graphene. Physical Chemistry Chemical Physics, 2015, 17, 12778-12785. | 1.3 | 17 |
| 75 | A comparison of neutral and charged species of one- and two-dimensional models of graphene nanoribbons using multireference theory. Journal of Chemical Physics, 2015, 142, 054302. | 1.2 | 15 |
| 76 | Concave or convex Ï€-dimers: the role of the pancake bond in substituted phenalenyl radical dimers. Physical Chemistry Chemical Physics, 2015, 17, 23963-23969. | 1.3 | 40 |
| 77 | Hydrogen Abstraction from the Hydrazine Molecule by an Oxygen Atom. Journal of Physical Chemistry A, 2015, 119, 1628-1635. | 1.1 | 12 |
| 78 | Thermochemical and Kinetics of Hydrazine Dehydrogenation by an Oxygen Atom in Hydrazine-Rich Systems: A Dimer Model. Journal of Physical Chemistry A, 2015, 119, 12607-12614. | 1.1 | 7 |
| 79 | A Multireference Configuration Interaction Study of the Photodynamics of Nitroethylene. Journal of Physical Chemistry A, 2014, 118, 12011-12020. | 1.1 | 7 |
| 80 | Study of the Diradicaloid Character in a Prototypical Pancakeâ€Bonded Dimer: The Stacked Tetracyanoethylene (TCNE) Anion Dimer and the Neutral K<sub>2</sub>TCNE<sub>2</sub> Complex. ChemPhysChem, 2014, 15, 165-176. | 1.0 | 43 |
| 81 | Perturbational treatment of spin-orbit coupling for generally applicable high-level multi-reference methods. Journal of Chemical Physics, 2014, 141, 074105. | 1.2 | 33 |
| 82 | The Diverse Manifold of Electronic States Generated by a Single Carbon Defect in a Graphene Sheet: Multireference Calculations Using a Pyrene Defect Model. ChemPhysChem, 2014, 15, 3334-3341. | 1.0 | 10 |
| 83 | Nonadiabatic dynamics study of methaniminium with ORMAS: Challenges of incomplete active spaces in dynamics simulations. Computational and Theoretical Chemistry, 2014, 1040-1041, 158-166. | 1.1 | 6 |
| 84 | Radical sites in humic acids: A theoretical study on protocatechuic and gallic acids. Computational and Theoretical Chemistry, 2014, 1032, 42-49. | 1.1 | 22 |
| 85 | Comparison of multireference configuration interaction potential energy surfaces for HÂ+ÂO2Âà†'ÂHO2: the effect of internal contraction. Theoretical Chemistry Accounts, 2014, 133, 1. | 0.5 | 21 |
| 86 | Proton transfer processes in polar regions of humic substances initiated by aqueous aluminum cation bridges: A computational study. Geoderma, 2014, 213, 115-123. | 2.3 | 12 |
| 87 | Intermolecular interactions and charge transfer transitions in aromatic hydrocarbonâ€"tetracyanoethylene complexes. Physical Chemistry Chemical Physics, 2014, 16, 20586-20597. | 1.3 | 43 |
| 88 | Double Pancake Bonds: Pushing the Limits of Strong Ï€â€"Ï€ Stacking Interactions. Journal of the American Chemical Society, 2014, 136, 12958-12965. | 6.6 | 74 |
| 89 | Electronic Excitation Processes in Single-Strand and Double-Strand DNA: A Computational Approach. Topics in Current Chemistry, 2014, 356, 1-37. | 4.0 | 20 |
| 90 | Surface Hopping Dynamics with Correlated Single-Reference Methods: 9H-Adenine as a Case Study. Journal of Chemical Theory and Computation, 2014, 10, 1395-1405. | 2.3 | 170 |

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| 91 | A comparison of singlet and triplet states for one- and two-dimensional graphene nanoribbons using multireference theory. Theoretical Chemistry Accounts, 2014, 133, 1. | 0.5 | 56 |
| 92 | Rotational Barrier in Phenalenyl Neutral Radical Dimer: Separating Pancake and van der Waals Interactions. Journal of the American Chemical Society, 2014, 136, 5539-5542. | 6.6 | 120 |
| 93 | Direct Dynamics Simulation of the Activation and Dissociation of 1,5-Dinitrobiuret (HDNB). Journal of Physical Chemistry A, 2014, 118, 2228-2236. | 1.1 | 12 |
| 94 | Comparison of LC-TDDFT and ADC(2) Methods in Computations of Bright and Charge Transfer States in Stacked Oligothiophenes. Journal of Chemical Theory and Computation, 2014, 10, 3280-3289. | 2.3 | 54 |
| 95 | Newtonâ€<scp>X</scp>: a surfaceâ€hopping program for nonadiabatic molecular dynamics. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 26-33. | 6.2 | 370 |
| 96 | Molecular Models of Cation and Water Molecule Bridges in Humic Substances. , 2014, , 107-115. | | 4 |
| 97 | Ab Initio Modeling of Excitonic and Charge-Transfer States in Organic Semiconductors: The PTB1/PCBM Low Band Gap System. Journal of the American Chemical Society, 2013, 135, 18252-18255. | 6.6 | 59 |
| 98 | Comparison of Cluster, Slab, and Analytic Potential Models for the Dimethyl Methylphosphonate (DMMP)/TiO<sub>2</sub>(110) Intermolecular Interaction. Journal of Physical Chemistry C, 2013, 117, 17613-17622. | 1.5 | 18 |
| 99 | Multiscale Simulation of the Ground and Photo-Induced Charge-Separated States of a Molecular Triad in Polar Organic Solvent: Exploring the Conformations, Fluctuations, and Free Energy Landscapes. Journal of Physical Chemistry B, 2013, 117, 12065-12075. | 1.2 | 21 |
| 100 | The effect of dimerization on the excited state behavior of methylated xanthine derivatives: a computational study. Photochemical and Photobiological Sciences, 2013, 12, 1496. | 1.6 | 5 |
| 101 | Electronic excitation and structural relaxation of the adenine dinucleotide in gas phase and solution. Photochemical and Photobiological Sciences, 2013, 12, 1440-1452. | 1.6 | 46 |
| 102 | The Multiradical Character of Oneâ€and Twoâ€Dimensional Graphene Nanoribbons. Angewandte Chemie - International Edition, 2013, 52, 2581-2584. | 7.2 | 197 |
| 103 | Synthesis, Spectroscopy, and Computational Analysis of Photoluminescent Bis(aminophenyl)â€Substituted Thiophene Derivatives. ChemPhysChem, 2013, 14, 1016-1024. | 1.0 | 18 |
| 104 | Nonadiabatic Photodynamics of a Retinal Model in Polar and Nonpolar Environment. Journal of Physical Chemistry A, 2013, 117, 2790-2799. | 1.1 | 55 |
| 105 | Electronically Excited States in Poly(p-phenylenevinylene): Vertical Excitations and Torsional Potentials from High-Level Ab Initio Calculations. Journal of Physical Chemistry A, 2013, 117, 2181-2189. | 1.1 | 65 |
| 106 | Ultrafast non-adiabatic dynamics of ethylene including Rydberg states. Molecular Physics, 2013, 111, 2439-2450. | 0.8 | 41 |
| 107 | Cis-transphotoisomerization of azobenzene upon excitation to the S<sub>1</sub>state: an ab initio molecular dynamics and QM/MM study. Proceedings of SPIE, 2012, , . | 0.8 | 2 |
| 108 | OÂ+ÂC2H4 potential energy surface: lowest-lying singlet at the multireference level. Theoretical Chemistry Accounts, 2012, 131, 1. | 0.5 | 5 |

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| 109 | Surface hopping dynamics using a locally diabatic formalism: Charge transfer in the ethylene dimer cation and excited state dynamics in the 2-pyridone dimer. Journal of Chemical Physics, 2012, 137, 22A514. | 1.2 | 173 |
| 110 | Multiconfiguration Self-Consistent Field and Multireference Configuration Interaction Methods and Applications. Chemical Reviews, 2012, 112, 108-181. | 23.0 | 559 |
| 111 | The stability of the acetic acid dimer in microhydrated environments and in aqueous solution. Physical Chemistry Chemical Physics, 2012, 14, 4162. | 1.3 | 18 |
| 112 | Critical appraisal of excited state nonadiabatic dynamics simulations of 9H-adenine. Journal of Chemical Physics, 2012, 137, 22A503. | 1.2 | 102 |
| 113 | Laser pulse trains for controlling excited state dynamics of adenine in water. Physical Chemistry Chemical Physics, 2012, 14, 4687. | 1.3 | 23 |
| 114 | Strikingly Different Effects of Hydrogen Bonding on the Photodynamics of Individual Nucleobases in DNA: Comparison of Guanine and Cytosine. Journal of the American Chemical Society, 2012, 134, 13662-13669. | 6.6 | 31 |
| 115 | Direct dynamics simulation of dioxetane formation and decomposition via the singlet Â·Oâ€“Oâ€“CH2â€“CH2Â· biradical: Non-RRKM dynamics. Journal of Chemical Physics, 2012, 137, 044305. | 1.2 | 22 |
| 116 | QM/MM non-adiabatic decay dynamics of formamide in polar and non-polar solvents. Physical Chemistry Chemical Physics, 2012, 14, 13262. | 1.3 | 11 |
| 117 | Analysis of Excitonic and Charge Transfer Interactions from Quantum Chemical Calculations. Journal of Chemical Theory and Computation, 2012, 8, 2777-2789. | 2.3 | 375 |
| 118 | Non-adiabatic excited state dynamics of riboflavin after photoexcitation. Physical Chemistry Chemical Physics, 2012, 14, 8693. | 1.3 | 21 |
| 119 | UV Absorption Spectrum of Alternating DNA Duplexes. Analysis of Excitonic and Charge Transfer Interactions. Journal of Physical Chemistry A, 2012, 116, 11151-11160. | 1.1 | 70 |
| 120 | Electronic spectra of nitroethylene. International Journal of Quantum Chemistry, 2012, 112, 1225-1232. | 1.0 | 10 |
| 121 | Model Systems for Dynamics of Ï€-Conjugated Biomolecules in Excited States. , 2012, , 1175-1213. | | 3 |
| 122 | The effect of hydrogen bonding on the excited-state proton transfer in 2-(2â€²-hydroxyphenyl)benzothiazole: a TDDFT molecular dynamics study. Physical Chemistry Chemical Physics, 2012, 14, 9016. | 1.3 | 69 |
| 123 | OÂ+ÂC2H4 potential energy surface: excited states and biradicals at the multireference level. Theoretical Chemistry Accounts, 2012, 131, 1. | 0.5 | 8 |
| 124 | Proton exchange reactions of C2â€“C4 alkanes sorbed in ZSM-5 zeolite. Theoretical Chemistry Accounts, 2012, 131, 1. | 0.5 | 11 |
| 125 | Electronically excited states and photodynamics: a continuing challenge. Theoretical Chemistry Accounts, 2012, 131, 1. | 0.5 | 77 |
| 126 | Electronically excited states and photodynamics: a continuing challenge. , 2012, , 147-160. | | 1 |

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| 127 | Methyl and Pentyl Chloride in a Microhydrated Environment and at the Liquid Waterâ^'Vapor Interface: A Theoretical Study. Journal of Physical Chemistry B, 2011, 115, 1807-1816. | 1.2 | 8 |
| 128 | Molecular Dynamics Simulations of Water Molecule-Bridges in Polar Domains of Humic Acids. Environmental Science & Technology, 2011, 45, 8411-8419. | 4.6 | 54 |
| 129 | Excited-State Intermolecular Proton Transfer Reactions of 7-Azaindole(MeOH)<sub>n</sub> (n = 1â€“3) Clusters in the Gas phase: On-the-Fly Dynamics Simulation. Journal of Physical Chemistry A, 2011, 115, 14129-14136. | 1.1 | 45 |
| 130 | Computational and Methodological Elements for Nonadiabatic Trajectory Dynamics Simulations of Molecules. Advanced Series in Physical Chemistry, 2011, , 415-462. | 1.5 | 18 |
| 131 | Photodynamical simulations of cytosine: characterization of the ultrafast bi-exponential UV deactivation. Physical Chemistry Chemical Physics, 2011, 13, 6145. | 1.3 | 84 |
| 132 | Nonadiabatic Dynamics of Uracil: Population Split among Different Decay Mechanisms. Journal of Physical Chemistry A, 2011, 115, 5247-5255. | 1.1 | 84 |
| 133 | The decay mechanism of photoexcited guanine â^' A nonadiabatic dynamics study. Journal of Chemical Physics, 2011, 134, 014304. | 1.2 | 70 |
| 134 | Semiclassical dynamics simulations of charge transport in stacked Ï€-systems. Journal of Chemical Physics, 2011, 134, 034309. | 1.2 | 27 |
| 135 | Nonadiabatic Molecular Dynamics Study of the cisâ€“trans Photoisomerization of Azobenzene Excited to the S<sub>1</sub> State. Journal of Physical Chemistry A, 2011, 115, 11136-11143. | 1.1 | 109 |
| 136 | Study of solvent effect on the stability of water bridge-linked carboxyl groups in humic acid models. Geoderma, 2011, 169, 20-26. | 2.3 | 26 |
| 137 | Wettability of kaolinite (001) surfaces â€" Molecular dynamic study. Geoderma, 2011, 169, 47-54. | 2.3 | 176 |
| 138 | Absorption and Fluorescence of PRODAN in Phospholipid Bilayers: A Combined Quantum Mechanics and Classical Molecular Dynamics Study. Journal of Physical Chemistry A, 2011, 115, 11428-11437. | 1.1 | 43 |
| 139 | Columbusâ€"a program system for advanced multireference theory calculations. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 191-199. | 6.2 | 171 |
| 140 | Sorption of Selected Aromatic Substancesâ€"Application of Kinetic Concepts and Quantum Mechanical Modeling. Water, Air, and Soil Pollution, 2011, 215, 449-464. | 1.1 | 4 |
| 141 | Theoretical study of the excitation spectrum of azomethane. Chemical Physics, 2011, 380, 9-16. | 0.9 | 13 |
| 142 | The functionality of cation bridges for binding polar groups in soil aggregates. International Journal of Quantum Chemistry, 2011, 111, 1531-1542. | 1.0 | 46 |
| 143 | Influence of the active space on CASSCF nonadiabatic dynamics simulations. International Journal of Quantum Chemistry, 2011, 111, 3307-3315. | 1.0 | 20 |
| 144 | The chargeâ€transfer states in a stacked nucleobase dimer complex: A benchmark study. Journal of Computational Chemistry, 2011, 32, 1217-1227. | 1.5 | 73 |

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| 145 | Photodynamics of the adenine model 4-aminopyrimidine embedded within double strand of DNA. Collection of Czechoslovak Chemical Communications, 2011, 76, 631-643. | 1.0 | 10 |
| 146 | A grid services cloud for molecular modelling workflows. International Journal of Web and Grid Services, 2010, 6, 176. | 0.4 | 10 |
| 147 | Formamide as the Model Compound for Photodissociation Studies of the Peptide Bond. Challenges and Advances in Computational Chemistry and Physics, 2010, , 77-106. | 0.6 | 7 |
| 148 | Singlet and triplet potential surfaces for the O2+C2H4 reaction. Journal of Chemical Physics, 2010, 133, 184306. | 1.2 | 17 |
| 149 | The photodynamics of 2,4-diaminopyrimidine in comparison with 4-aminopyrimidine: The effect of amino-substitution. Chemical Physics Letters, 2010, 497, 129-134. | 1.2 | 16 |
| 150 | Non-adiabatic dynamics of pyrrole: Dependence of deactivation mechanisms on the excitation energy. Chemical Physics, 2010, 375, 26-34. | 0.9 | 124 |
| 151 | The effect of hydration on the photo-deactivation pathways of 4-aminopyrimidine. Chemical Physics, 2010, 375, 110-117. | 0.9 | 14 |
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